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UNITARY GROUP TENSOR OPERATOR ALGEBRAS FOR MANY-ELECTRON SYSTEMS: I. CLEBSCH–GORDAN AND RACAH COEFFICIENTS

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Abstract

A basis for the Racah–Wigner algebra of irreducible representations of the unitary group U(n) that are pertinent to quantum chemical models of many-electron systems is developed. Standard Clebsch–Gordan coefficients and isoscalar factors (also called coupling factors or reduced Wigner coefficients) for both symmetric (S_N) and unitary [U(n)] groups are extended to transformation coefficients and corresponding isoscalar factors relating canonical Young–Yamanouchi or Gel'fand–Tsetlin bases to simple partitioned bases. All these different types of isoscalar factors are interrelated using the well-known reciprocity between the S_N and U(n) tensor representations, and general expressions relating these different factors are given. For the two-column representations characterizing the many-electron theory, detailed explicit expressions are presented for both the above-mentioned relationships and for all relevant U(n) isoscalar factors. Finally, U(n) Racah coefficients are introduced and explicit expressions derived for certain special classes of these coefficients.

1. Introduction

Since its introduction into quantum chemistry [1,2], the unitary group approach (UGA) [1,3,4] to many-electron systems has evolved into a very versatile formalism [5–18] which enables the construction of efficient algorithms for computations involving spin-adapted N-electron tensorial orbital product bases and the corresponding matrix elements of particle number conserving operators [5–24]. In its standard version, it exploits Gel'fand–Tsetlin (GT) bases [25] that are adapted to the canonical subgroup chain $U(n) \supset U(n-1) \supset \ldots \supset U(1)$, thus enabling one to formulate a convenient representation scheme for the generation of relevant tensor product spaces [1,6,26] and to construct matrix representatives of the Hamiltonian as a product of segment values [6–12,27,28] associated with each orbital level. The versatility and

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efficiency of these algorithms facilitated the design of various codes for large-scale configuration interaction (CI) calculations [19–24], which often provide benchmark results in the electronic structure theory of small and medium-sized molecules. UGA formalism has also been employed in electron propagator theory [29], the coupled cluster approach [12,15,18,31], many-body perturbation theory (MBPT) [12,19], MC SCF approaches [32], and is being considered for relativistic effects (particularly the spin-orbit interaction) [33]. The UGA developments that were stimulated by the structure of the many-electron problem [1,5–7] can, in fact, be extended to the case of more general, more than two-column irreducible representations (irreps) [34,35] and be exploited in problems of nuclear structure and nuclear magnetic resonance spectroscopy. The principal features of UGA can thus be summarized as follows:

(i) UGA provides spin-adapted bases for the expansion of exact molecular orbital model wave functions that are suitable not only for CI expansions, but also in valence-bond theory [12], ligand field theory [36], nuclear shell model calculations [3], etc.

(ii) It enables an efficient computer storage for even very large basis sets, using the distinct row table (DRT) representation as well as convenient graphical representation of these bases [6,7,26].

(iii) Finally, it facilitates an efficient matrix element evaluation of U(n) generators and of their products, and thus of various physical observables [1,5–8,16,27,28].

The importance and usefulness of UGA for the quantum theory of molecular electronic structure stems primarily from the fact that all particle number conserving operators can be expressed in terms of U(n) generators. Thus, although the unitary group is *not* the invariance or symmetry group of the relevant model Hamiltonians, it may be regarded, in a certain sense, as a dynamical group [17,18]. This dynamical group viewpoint recently led to an extension of UGA, referred to as Clifford Algebra UGA (CAUGA) [13–15], through an embedding of U(n) into a much larger group U(2^n), whose fundamental representation states can be regarded as Clifford numbers spanning the Clifford algebra C_n. Moreover, the CAUGA group U(2^n) represents a true dynamical group for any n-orbital model, since all the states of such a model are contained within a single irreducible representation (irrep) $\langle 2\dot{0}\rangle \equiv \langle 2000\ldots 0\rangle$. In contrast to UGA, based on the GT chain, CAUGA admits arbitrary coupling schemes. We can thus employ canonical GT states as in UGA, or various partitioned bases [14] or valence bond (VB) states [13,14] which, in some sense, represent the most natural choice. This aspect of spin-adapted VB states was recently developed by Paldus et al. [37] and, from a different viewpoint, exploiting the so-called bonded tableaux, by Li and Zhang [38].

It is also important to emphasize the close relationship that exists between the unitary U(n), symmetric S_N, and angular momentum SU(2) groups. Indeed, any one of these groups can be successfully exploited in the electronic structure calculations, and

each brings a unique and useful viewpoint on the problem. Thus, the relationship between U(n) and SU(2) or S_N and SU(2) was successfully employed in deriving segmentation fomulas for generator product matrix elements [8,27] and, generally, for antisymmetrized-geminal product wave function formalism, particularly for spin bonded functions [28]. The UGA DRT structure was also successfully implemented at the S_N level [26,39], reflecting the well-known S_N–U(n) reciprocity, first established and employed in the pioneering work by Schur and Weyl.

It is our belief that a future development of UGA formalism can greatly benefit from an intimate understanding of the S_N–U(n) reciprocity and of the underlying mathematical structure, and will enable the development of a more general formalism which will closely parallel the SU(2) formalism and will be capable of handling non-canonical GT states, such as required in partitioned bases [14,40] as well as general particle number non-conserving [13,29,41] and/or spin-dependent [33] operators. It is the main goal of this series of papers to initiate these developments by introducing a unitary group tensor operator (Racah–Wigner) algebra that is particularly suitable for the quantum theory of many-electron systems. The angular momentum algebra $su(2)$, which will motivate present developments, was first introduced into quantum mechanics by Racah, Wigner and others and soon became a standard method in theoretical physics and chemistry. Racah–Wigner $su(2)$ algebra can be found in most advanced texts on quantum mechanics, as well as in numerous special monographs [42–47]. Today, it represents a standard tool in the many branches of theoretical physics and chemistry that require coupling of angular momenta. Various diagrammatic techniques, referred to as graphical methods of spin algebras, were developed for an efficient handling of these problems [48–50]. Numerous applications in collision theory, intermolecular forces and other fields come to mind. The same idea was also extended to finite point groups, and the resulting irreducible tensor method was developed in ligand field theory by Griffith [51].

The Racah–Wigner algebra for general unitary groups U(n) was also widely studied by Biedenham, Louck and others [52–59], and an authoritative monograph on these developments is now available [46,47]. Although many of these very ingenious mathematical advances await to be exploited in actual applications, the developments of the past decade in quantum chemistry clearly indicate the important role the unitary group can play. These developments can be further enhanced by exploiting a modern representation theory for semi-simple Lie algebras as developed by Harish–Chandra, Kostant, Verma and others [60], as recent work of Coleman [61] and Gould [62] indicates. In the future, we hope to investigate the close relationship that exists between the present $su(2)$-modelled approach and more general Green–Gould representation theory for unitary and orthogonal Lie groups [62–64].

Just as the appearance of the Wigner formula [65] for the SU(2) Clebsch–Gordan (CG) coefficients greatly benefited the development of the angular momentum calculus, there is little doubt that the development of the Racah–Wigner algebra for other groups, and particularly their applications, will require efficient computation of CG coefficients and closely related higher-order invariants, such as Racah coefficients, 9j symbols, etc.

for these groups. At present, a vast literature exists that deals with these topics for U(n) and that is based on very different approaches and viewpoints. To mention at least the most important ones, we note pattern calculus of Biedenharn and Louck [54], Racah's infinitesimal operator approach [66], diagonalization of a complete system of commuting operators (CSCO) [67], vector coherent state theory [68–70] and the build-up procedure for isoscalar factors [71]. For smaller groups, which are relevant in the theory of a few particle systems, Chen et al. [72a] developed an efficient code that determines the isoscalar factors for an arbitrary partition and produced their tables [72b,c]. Although these tables are extremely handy in various studies and developments, their general usefulness is rather limited in quantum chemical applications, where the order of the group n as well as the number of electrons N determining the general irrep [1] can be rather large. Thus, unlike the point group irreducible tensor methods for ligand field theory and similar applications, where such tables are essential [73], the large-scale calculations of molecular electronic structure require the availability of efficient algorithms for the relevant U(n) CG or Racah coefficients, which enable us to generate these quantities "on the fly". An additional advantage may result when these algorithms can be made n-independent, since n can be rather large and will change when going from one 1-electron basis (or model) to another. The feasibility of such a development was implied in recent papers [72,74,75] considering U(n) CG coefficients and related U(n) and S_N isoscalar factors.

In the general case, the major difficulty in an efficient construction of U(n) CG coefficients is the multiplicity problem. This problem has not yet been satisfactorily resolved within the group representation theory itself. It is fortunate, however, that in most cases which are relevant in applications to many-electron systems, the multiplicity problem can be avoided. For example, no multiplicity will arise when coupling two electronic GT states describing sub-systems with N_1 and N_2 electrons into a resulting $N = N_1 + N_2$ electron state. Consequently, the relevant CG coefficients can be completely determined and given by explicit closed formulas, just as in the SU(2) case.

In this paper, we present an algorithm for an efficient construction of CG coefficients for U(n) GT bases, as well as corresponding isoscalar factors (or reduced Wigner coefficients) and Racah coefficients. Although numerous results given in this paper hold for general U(n) irreps, the final explicit formulas are invariably given for two-column irreps that are relevant for many-electron problems. We start (section 2) with an overview of the outer product coupling coefficients and corresponding isoscalar factors for the symmetric group S_N, and extend these concepts to the case of transformations to partitioned bases. The resulting isoscalar factors are referred to as transformation (I_t) factors in order to distinguish them from standard isoscalar factors, which may also be called coupling factors. Analogous concepts are introduced in section 3 for the unitary groups. We then exploit the reciprocity between the S_N and U(n) irreps in section 4, obtaining the relationships between various isoscalar factors of sections 2 and 3. Relying entirely on the S_N representation theory, we derive explicit expressions for U(n) isoscalar factors involving two-column irreps. These resulting closed expressions are not only very simple, but also n-independent, since they result from symmetric group

considerations. They are presented in section 5, and their derivation is given in the appendix. Finally, in sections 6 and 7, we introduce U(n) Racah coefficients and derive formulas for certain important classes of these coefficients. In particular, some recent results obtained with the vector coherent state theory [70] are obtained in an equivalent but distinct form which is n-independent.

The results of this paper lay the ground for further development of tensor operator algebras, which will be given in a subsequent paper of this series.

2. Summary of the outer product coupling and basis transformation coefficients of the symmetric group S_N

2.1. BASIC CONCEPTS AND NOTATION

Consider an irreducible representation (irrep) $[\lambda]$ of S_N and its carrier space $\mathcal{V}_\lambda$. These irreps are uniquely labeled by Young diagrams $[\lambda]$, $[\lambda] \equiv [\lambda_1 \lambda_2, \ldots, \lambda_N]$, $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_N$, with $\{\lambda_i\}$ representing a partition of N,

$$\sum_{i=1}^{N} \lambda_i = N. \tag{1}$$

Throughout this paper, we designate the irreps by lower case Greek letters λ, μ, ν, etc. Any relationship or expression using this notation is valid generally for an *arbitrary* irrep of S_N [or U(n)]. Later, when we restrict our considerations to at most two-column tableaux that are relevant for many-electron systems, the irreps are labeled explicitly as $[2^a 1^b]$, or $\langle 2^a 1^b \rangle$ for U(n), or simply (a, b). The dimension of $[\lambda]$, $\dim[\lambda] = \dim \mathcal{V}_\lambda =: f_\lambda$, is easily obtained in terms of hook lengths h_i as [76,77]

$$f_\lambda = N! / \prod_i h_i . \tag{2}$$

It is also well known that we can label the *standard* or *canonical* Young–Yamanouchi (YY) basis for $[\lambda]$, which is adapted to the chain

$$S_N \supset S_{N-1} \supset \ldots \supset S_3 \supset S_2 \supset S_1, \tag{3}$$

by $|[\lambda] r\rangle$, where r designates either a Young tableau or a Yamanouchi symbol $r \equiv r_N r_{N-1}, \ldots, r_1$ [78]. We shall also employ a *nonstandard* basis, which is adapted to the chain

$$S_N \supset S_{N_1} \times S_{N_2}, \quad N = N_1 + N_2, \tag{4}$$

and which is canonical with respect to both S_{N_1} and S_{N_2}, designating its vectors by the symbol

$$|[\lambda]r^1r^2\rangle \equiv |[\lambda];[\lambda_1]r^1,[\lambda_2]r^2\rangle, \tag{5}$$

where $[\lambda_1]$ and $[\lambda_2]$ are S_{N_1} and S_{N_2} irreps and r^1 and r^2 are adapted to the canonical chains

$$S_{N_1} \supset S_{N_1-1} \supset \ldots \supset S_1 \quad \text{and} \quad S_{N_2} \supset S_{N_2-1} \supset \ldots \supset S_1, \tag{6}$$

respectively. It will sometimes also be convenient to label standard basis vectors $|[\lambda]r\rangle$ as

$$|[\lambda]r\rangle \equiv |[\lambda]r^1\rho^2\rangle, \tag{7}$$

where r^1 is a partial Young tableau containing the first N_1 indices $1, 2, \ldots, N_1$, while ρ^2, which is generally a nonstandard sub-tableau, consists of the remaining N_2 indices $N_1 + 1, N_1 + 2, \ldots, N_1 + N_2 = N$. Thus, for example, for the first YY basis vector of the irrep $[2^21]$ of S_5 (using canonical ordering)

$$\left| \begin{array}{cc} & 1 \quad 2 \\ [2^21] & 3 \quad 4 \\ & 5 \end{array} \right\rangle \equiv |[2^21]\ 3,2,2,1,1\rangle = |[2^21]r^1\rho^2\rangle, \tag{8}$$

when choosing $N_1 = 3$ and $N_2 = 2$, we have

$$r^1 = \begin{array}{cc} 1 & 2 \\ 3 & \end{array}, \quad \rho^2 = \begin{array}{cc} \cdot & 4 \\ 5 & \end{array}. \tag{9}$$

We shall always use letters of the Greek alphabet to label the second (generally non-standard) sub-tableau in order to avoid confusion with the shorthand notation for a non-standard basis shown on the left-hand side of eq. (5). Also, for the sake of easier typesetting, we do not draw boxes around the individual entries in Young and Weyl tableaux unless confusion is possible.

It is clear from eqs. (4)–(6) that it will be useful to generalize the concept of a permutation P, representing a map $P: i \to P(i)$ from $\{1, 2, \ldots, N\}$ onto itself, to a more general ordered set ω,

$$\omega = \{i_1, i_2, \ldots, i_N\}, \qquad i_1 < i_2 < \ldots < i_N. \tag{10}$$

We thus introduce the generalized permutation group $S_N(\omega)$ defined as a set of all maps P of ω onto itself. The standard symmetric group S_N then corresponds to a special choice for ω, namely

$$\omega_0 \equiv \{1, 2, \ldots, N\}, \tag{11}$$

so that $S_N \equiv S_N(\omega_0)$. We can now define a *generalized standard basis* for $S_N(\omega)$ as a basis adapted to the chain

$$S_N(\omega) \supset S_{N-1}(\omega_{N-1}) \supset S_{N-2}(\omega_{N-2}) \supset \ldots \supset S_1(\omega_1), \tag{12}$$

where the family of ordered sets ω_i,

$$\omega \equiv \omega_N \supset \omega_{N-1} \supset \omega_{N-2} \supset \ldots \supset \omega_1, \tag{13}$$

is recursively generated by deleting the largest symbol at each step, i.e.

$$\omega_{j-1} := \omega_j \backslash \{i_j^{\max}\}, \tag{14}$$

where

$$i_j^{\max} = \max(\omega_j). \tag{15}$$

We are now ready to introduce an outer product basis for S_N. Let us consider an arbitrary partition of the set ω_0 (eq. (11)) into the two disjoint sets ω^1 and ω^2 with N_1 and N_2 objects, respectively, $N = N_1 + N_2$,

$$\omega^1 = \{i_1, i_2, \ldots, i_{N_1}\}, \quad i_1 < i_2 < \ldots < i_{N_1}, \tag{16a}$$

$$\omega^2 = \{j_1, j_2, \ldots, j_{N_2}\}, \quad j_1 < j_2 < \ldots < j_{N_2}, \tag{16b}$$

so that

$$\omega^1 \cup \omega^2 = \omega_0 = \{1, 2, \ldots, N\}, \qquad \omega^1 \cap \omega^2 = \varnothing. \tag{17}$$

These sets define two generalized symmetric groups $S_{N_1}(\omega^1)$ and $S_{N_2}(\omega^2)$. Introducing the following maps

$$\begin{bmatrix} \omega_0^1 \\ \omega^1 \end{bmatrix} = \begin{bmatrix} 1 & 2 & \ldots & N_1 \\ i_1 & i_2 & \ldots & i_{N_1} \end{bmatrix}, \quad \begin{bmatrix} \omega_0^2 \\ \omega^2 \end{bmatrix} = \begin{bmatrix} N_1+1 & N_1+2 & \ldots & N \\ j_1 & j_2 & \ldots & j_{N_2} \end{bmatrix}, \tag{18}$$

we can obtain generalized standard bases for $S_{N_1}(\omega^1)$ and $S_{N_2}(\omega^2)$ by applying these maps to standard bases for S_{N_1} and $S_{N_2} \approx S_{N_2}(\omega_0^2)$, respectively, namely

$$|[\lambda_1]r^1(\omega^1)\rangle = \begin{bmatrix} \omega_0^1 \\ \omega^1 \end{bmatrix} |[\lambda_1]r^1(\omega_0^1)\rangle \equiv \begin{bmatrix} \omega_0^1 \\ \omega^1 \end{bmatrix} |[\lambda_1]r^1\rangle, \tag{19a}$$

and

$$|[\lambda_2]r^2(\omega^2)\rangle = \begin{bmatrix} \omega_0^2 \\ \omega^2 \end{bmatrix} |[\lambda_2]r^2\rangle, \tag{19b}$$

where all the labels in the Young tableau r^2 have been shifted by N_1. Generally, $r^k(\omega^k)$ designates a Young tableau in which the map

$$\begin{bmatrix} \omega_0^k \\ \omega^k \end{bmatrix} : j \rightarrow l_j$$

(eq. (18)) has been carried out, so that $r^k \equiv r^k(\omega_0^k)$. Clearly, r^k remains unchanged when the Yamanouchi symbol notation is used. It must be stressed that although the maps (18) are not permutations, their composition is a permutation assuming that eq. (17) holds, i.e.

$$\begin{bmatrix} \omega_0^1 \\ \omega^1 \end{bmatrix} \circ \begin{bmatrix} \omega_0^2 \\ \omega^2 \end{bmatrix} = \begin{bmatrix} \omega_0^2 \\ \omega^2 \end{bmatrix} \circ \begin{bmatrix} \omega_0^1 \\ \omega^1 \end{bmatrix} = \begin{pmatrix} \omega_0^1 & \omega_0^2 \\ \omega^1 & \omega^2 \end{pmatrix}. \tag{20}$$

The tensor product of generalized standard bases

$$|[\lambda_1]r^1(\omega^1)\rangle \otimes |[\lambda_2]r^2(\omega^2)\rangle \equiv |[\lambda_1]r^1(\omega^1)\rangle\,|\,[\lambda_2]r^2(\omega^2)\rangle \tag{21}$$

for all possible choices of ω^1 and ω^2 satisfying eqs. (16) and (17) is referred to as a *standard outer product basis* for S_N. For each *fixed* choice of ω^1 and ω^2, the basis (21) provides an irrep of $S_{N_1} \times S_{N_2}$. However, considering *all possible* partitions of ω into ω^1 and ω^2 (eqs. (16) and (17)), we obtain a reducible representation for S_N of the dimension D,

$$D([\lambda_1] \otimes [\lambda_2]) = N! f_{\lambda_1} f_{\lambda_2} / (N_1! N_2!) = \binom{N}{N_1} f_{\lambda_1} f_{\lambda_2}, \tag{22}$$

where f_{λ_k} is the dimension of $[\lambda_k]$ of S_{N_k}, $k = 1, 2$, given by eq. (2). We shall next outline the relationship between these various irrep bases.

2.2. OUTER PRODUCT COUPLING COEFFICIENTS AND NONSTANDARD BASIS TRANSFORMATION COEFFICIENTS

Forming appropriate linear combinations of basis states (21) will yield standard bases for S_N. The relevant *outer product coupling coefficients*, which achieve this transformation, are defined as follows:

$$|[\lambda]m\rangle = \sum_{r^1,r^2} \sum_{\omega^1,\omega^2} \langle [\lambda_1]r^1(\omega^1), [\lambda_2]r^2(\omega^2) \,|\, [\lambda]m\rangle \,|\, [\lambda_1]r^1(\omega^1)\rangle \,|\, [\lambda_2]r^2(\omega^2)\rangle, \quad (23)$$

where $|[\lambda]m\rangle$ form an arbitrary orthonormal basis for the irrep $[\lambda]$ of S_N. In the following, we shall pay special attention to standard bases for S_N, in which case

$$|[\lambda]m\rangle = |[\lambda]r\rangle. \quad (24)$$

Note that the "partitioned" notation of eq. (7) will only be useful for those terms on the right-hand side of eq. (23), which correspond to standard partitioning of ω into ω_0^1 and ω_0^2. In view of the orthogonality of both bases related by eq. (23), the outer product coupling coefficients define a unitary transformation and satisfy the same orthogonality relations as the usual Clebsch–Gordan coefficients of the SU(2). These can be employed to invert the transformation (23), obtaining

$$|[\lambda_1]r^1(\omega^1)\rangle \,|\, [\lambda_2]r^2(\omega^2)\rangle \equiv |[\lambda_1]r^1(\omega^1);[\lambda_2]r^2(\omega^2)\rangle$$

$$= \sum_{[\lambda],m} |[\lambda]m\rangle\langle[\lambda]m \,|\, [\lambda_1]r^1(\omega^1), [\lambda_2]r^2(\omega^2)\rangle. \quad (23')$$

Considering an arbitrary matrix element of some permutation $P \in S_N$ in the outer product basis, we easily find, using eq. (23′) and the great orthogonality relations for an orthogonal irrep $D^{[\lambda]}(P)_{\tilde{m},m} \equiv \langle[\lambda]\tilde{m}\,|P\,|[\lambda]m\rangle$ of S_N, that the outer product coefficients possess the following useful property

$$\langle [\lambda_1]\tilde{r}^1(\tilde{\omega}^1), [\lambda_2]\tilde{r}^2(\tilde{\omega}^2) \,|\, [\lambda]\tilde{m}\rangle\langle[\lambda]m \,|\, [\lambda_1]r^1(\omega^1), [\lambda_2]r^2(\omega^2)\rangle$$

$$= \frac{f_\lambda}{N!} \sum_{P\in S_N} D^{[\lambda]}(P)_{\tilde{m},m} \langle [\lambda_1]\tilde{r}^1(\tilde{\omega}^1), [\lambda_2]\tilde{r}^2(\tilde{\omega}^2) \,|P|\, [\lambda_1]r^1(\omega^1), [\lambda_2]r^2(\omega^2)\rangle. \quad (25)$$

In order to achieve a transition to standard labeling as given by ω_0^1 and ω_0^2, we observe that in a coset decomposition of S_N with respect to its subgroup $S_{N_1} \times S_{N_2}$, $N = N_1 + N_2$, i.e.

$$S_N = \bigcup_{Q_\omega} Q_\omega (S_{N_1} \times S_{N_2}), \quad (26)$$

we can always choose Q_ω to be of the form

$$Q_\omega = \begin{pmatrix} \omega_0^1 & \omega_0^2 \\ \omega^1 & \omega^2 \end{pmatrix} = \begin{bmatrix} \omega_0^1 \\ \omega^1 \end{bmatrix} \circ \begin{bmatrix} \omega_0^2 \\ \omega^2 \end{bmatrix}, \quad (27)$$

assuming that $S_{N_1} = S_{N_1}(\omega_0^1)$ and $S_{N_2} = S_{N_2}(\omega_0^2)$. Thus, for example, decomposing S_4 with respect to $S_2 \times S_2 \equiv S_2\{1,2\} \times S_2\{3,4\}$, we obtain six cosets (since $4!/2! \times 2! = 6$), each containing four elements, as shown in table 1. Although it would be most natural to choose the permutations given in the first column as coset representatives, we have to make another choice if we wish eqs. (26) and (27) to hold, as indicated in table 1.

Table 1

Coset decomposition of S_4 with respect to $S_2 \times S_2$ and suitable coset representatives Q_ω of the form (27). The last column gives the sets ω^1 and ω^2 appearing in the decomposition of eq. (27)

Cosets				Q_ω	$\omega^1;\omega^2$
(1),	(12),	(34),	(12)(34)	(1)	{1,2};{3,4}
(13),	(123),	(134),	(1234)	(123)	{2,3};{1,4}
(23),	(132),	(234),	(1342)	(23)	{1,3};{2,4}
(14),	(124),	(143),	(1243)	(1243)	{2,4};{1,3}
(24),	(142),	(243),	(2143)	(243)	{1,4};{2,3}
(1324),	(14)(23),	(13)(24),	(1423)	(13)(24)	{3,4};{1,2}

With such a decomposition in hand, we can express the outer product basis states (21) in terms of standard outer product states associated with subsets ω_0^1 and ω_0^2, namely

$$|[\lambda_1]r^1(\omega^1)\rangle\,|[\lambda_2]r^2(\omega^2)\rangle = Q_\omega |[\lambda_1]r^1(\omega_0^1)\rangle\,|[\lambda_2]r^2(\omega_0^2)\rangle. \tag{28}$$

Setting now ω^1 and ω^2 in eq. (25) equal to ω_0^1 and ω_0^2, respectively, and exploiting the decomposition (26), we can rewrite the right-hand side of (25) as

$$\begin{aligned}
&\frac{f_\lambda}{N!} \sum_{P_1 \in S_{N_1}} \sum_{P_2 \in S_{N_2}} \sum_{Q_\omega} D^{[\lambda]}(Q_\omega P_1 P_2)_{\tilde{m},m} \\
&\times \langle [\lambda_1]\tilde{r}^1(\tilde{\omega}^1);[\lambda_2]\tilde{r}^2(\tilde{\omega}^2)\,|\,Q_\omega P_1 P_2\,|\,[\lambda_1]r^1(\omega_0^1);[\lambda_2]r^2(\omega_0^2)\rangle \\
&= \frac{f_\lambda}{N!} \sum_{P_1} \sum_{P_2} \sum_{Q_\omega} D^{[\lambda]}(Q_\omega P_1 P_2)_{\tilde{m},m} \\
&\sum_{s^1,s^2} \langle [\lambda_1]\tilde{r}^1(\tilde{\omega}^1);[\lambda_2]\tilde{r}^2(\tilde{\omega}^2)\,|\,Q_\omega\,|\,[\lambda_1]s^1(\omega_0^1);[\lambda_2]s^2(\omega_0^2)\rangle \\
&\times \langle [\lambda_1]s^1(\omega_0^1)\,|\,P_1\,|\,[\lambda_1]r^1(\omega_0^1)\rangle \langle [\lambda_2]s^2(\omega_0^2)\,|\,P_2\,|\,[\lambda_2]r^2(\omega_0^2)\rangle.
\end{aligned} \tag{29}$$

Clearly, the sum over Q_ω reduces to a single term $Q_{\tilde{\omega}}$ which transforms ω_0 into $\tilde{\omega} \equiv \{\tilde{\omega}^1, \tilde{\omega}^2\}$, namely

$$Q_{\tilde{\omega}}\omega_0 = \tilde{\omega}, \tag{30}$$

in which case the matrix element over Q_{ω} reduces to a product of Kronecker deltas for Young tableaux (or Yamanouchi symbols)

$$\delta_{\tilde{r}^1,s^1}\,\delta_{\tilde{r}^2,s^2}.$$

We thus finally obtain the desired relationship

$$\langle [\lambda_1]\tilde{r}^1(\tilde{\omega}^1), [\lambda_2]\tilde{r}^2(\tilde{\omega}^2)\,|\,[\lambda]\tilde{m}\rangle\langle [\lambda]m\,|\,[\lambda_1]r^1(\omega_0^1), [\lambda_2]r^2(\omega_0^2)\rangle$$
$$= \frac{f_\lambda}{N!}\sum_{P_1\in S_{N_1}}\sum_{P_2\in S_{N_2}} D^{[\lambda]}(Q_{\tilde{\omega}}P_1P_2)_{\tilde{m},m}D^{[\lambda_1]}(P_1)_{\tilde{r}^1,r^1}D^{[\lambda_2]}(P_2)_{\tilde{r}^2,r^2}, \tag{31}$$

where $\tilde{\omega}$ is defined by eq. (30). Setting, finally, $\tilde{\omega} = \omega_0$, so that $Q_{\tilde{\omega}} = (1) \equiv e$, and using the fact that $[\lambda]\downarrow S_{N_1} = [\lambda_1]$ (note that the multiplicity of $[\lambda_1]$ in $[\lambda]$ equals one), we can exploit the great orthogonality theorem for S_{N_1}, obtaining

$$\langle [\lambda_1]\tilde{r}^1(\omega_0^1), [\lambda_2]\tilde{r}^2(\omega_0^2)\,|\,[\lambda]\tilde{m}\rangle\langle [\lambda]m\,|\,[\lambda_1]r^1(\omega_0^1), [\lambda_2]r^2(\omega_0^2)\rangle$$
$$= \frac{N_1!f_\lambda}{N!f_{\lambda_1}}\sum_{P_2\in S_{N_2}} D^{[\lambda_2]}(P_2)_{\tilde{r}^2,r^2}\langle [\lambda]r^1\tilde{\rho}^2\,|P_2|\,[\lambda]r^1\rho^2\rangle, \tag{32}$$

where we also used the fact that when $|[\lambda]m\rangle = |[\lambda]r^1\rho^2\rangle$, then $|[\lambda]\tilde{m}\rangle = |[\lambda]\tilde{r}^1\tilde{\rho}^2\rangle$ must equal $|[\lambda]r^1\tilde{\rho}^2\rangle$, so that we must identify r^1 and $\tilde{r}^1$. This also implies that the outer product coupling coefficients are independent of r^1 or $\tilde{r}^1$, namely

$$\langle [\lambda_1]r^1(\omega_0^1), [\lambda_2]\tilde{r}^2(\omega_0^2)\,|\,[\lambda]r^1\rho^2\rangle = \langle [\lambda_1]\tilde{r}^1(\omega_0^1), [\lambda_2]\tilde{r}^2(\omega_0^2)\,|\,[\lambda]\tilde{r}^1\rho^2\rangle. \tag{33}$$

We now turn our attention to a transformation of a nonstandard basis $|[\lambda]r^1r^2\rangle$ (eq. (5)) to the standard basis for S_N. This is achieved by introducing the (nonstandard basis) *transfomation coefficients* defined as follows (note that the shorthand notation suppressing the irrep labels $[\lambda_1]$ and $[\lambda_2]$ (eq. (5)) is employed here and in the following text):

$$|[\lambda]r\rangle \equiv |[\lambda]r^1\rho^2\rangle = \sum_{[\lambda_2],r^2}\langle [\lambda]r^1r^2\,|\,[\lambda]r\rangle\,|\,[\lambda]r^1r^2\rangle, \tag{34}$$

or, conversely

$$|[\lambda]r^1r^2\rangle \equiv |[\lambda];[\lambda_1]r^1,[\lambda_2]r^2\rangle$$

$$= \sum_{\rho^2}\langle[\lambda]r^1\rho^2|[\lambda]r^1r^2\rangle|[\lambda]r^1\rho^2\rangle, \tag{35}$$

since these coefficients must satisfy the obvious orthonormality properties

$$\sum_{\rho^2}\langle[\lambda]r^1r^2|[\lambda]r^1\rho^2\rangle\langle[\lambda]r^1\rho^2|[\tilde{\lambda}]\tilde{r}^1\tilde{r}^2\rangle = \delta_{\lambda\tilde{\lambda}}\delta_{r^1\tilde{r}^1}\delta_{r^2\tilde{r}^2}, \tag{36}$$

and

$$\sum_{[\lambda_2]r_2}\langle[\lambda]r|[\lambda];[\lambda_1]r^1,[\lambda_2]r^2\rangle\langle[\lambda];[\lambda_1]r^1,[\lambda_2]r^2|[\tilde{\lambda}]\tilde{r}\rangle = \delta_{\lambda\tilde{\lambda}}\delta_{r\tilde{r}}\,. \tag{36'}$$

These coefficients are in fact closely related to the outer product coupling coefficients, as we shall now indicate. The key to this relationship is the fact that, up to a normalization factor $\mathcal{N}$, we can obtain the nonstandard basis vector (5) by projecting the standard basis vector $|[\lambda]r\rangle \equiv |[\lambda]r^1\tilde{\rho}^2\rangle$ with the S_{N_2} Young orthonormal unit $o^{[\lambda_2]}_{r^2\tilde{r}^2}$ associated with irrep $[\lambda_2]$, so that

$$\mathcal{N}|[\lambda]r^1r^2\rangle = o^{[\lambda_2]}_{r^2\tilde{r}^2}|[\lambda]r^1\tilde{\rho}^2\rangle, \tag{37}$$

where explicitly

$$o^{[\lambda_2]}_{r^2\tilde{r}^2} = \frac{f_{\lambda_2}}{N_2!}\sum_{P_2\in S_{N_2}} D^{[\lambda_2]}(P_2)_{r^2\tilde{r}^2}P_2\,. \tag{38}$$

We recall that these units possess the well-known algebraic orthogonality properties

$$o^{[\lambda]}_{rs}\,o^{[\mu]}_{tu} = \delta_{\lambda\mu}\delta_{st}\,o^{[\lambda]}_{ru}\,, \tag{39}$$

as well as the hermiticity property

$$o^{[\lambda]\dagger}_{rs} = o^{[\lambda]}_{sr}\,, \tag{40}$$

and that the second index $\tilde{r}^2$ is arbitrary as far as the projection property (eq. (37)) is concerned. Using the hermiticity property (eq. (40)), we see immediately that

$$\mathcal{N} = \langle[\lambda]r^1r^2|o^{[\lambda_2]}_{r^2\tilde{r}^2}|[\lambda]r^1\tilde{\rho}^2\rangle = \langle[\lambda]r^1\tilde{r}^2|[\lambda]r^1\tilde{\rho}^2\rangle, \tag{41}$$

so that projecting eq. (37) onto $|[\lambda]r\rangle = |[\lambda]r^1\rho^2\rangle$, we find that

$$\langle[\lambda]r^1\bar{r}^2|[\lambda]r^1\bar{\rho}^2\rangle\langle[\lambda]r^1\rho^2|[\lambda]r^1r^2\rangle$$
$$= \frac{f_{\lambda_2}}{N_2!}\sum_{P_2\in S_{N_2}} D^{[\lambda_2]}(P_2)_{r^2\bar{r}^2}\langle[\lambda]r^1\rho^2|P_2|[\lambda]r^1\bar{\rho}^2\rangle. \tag{42}$$

Comparing this relationship with the corresponding one for the outer product coupling coefficients (eq. (32)), we find that

$$\langle[\lambda_1]r^1(\omega_0^1),[\lambda_2]\bar{r}^2(\omega_0^2)|[\lambda]r^1\bar{\rho}^2\rangle\langle[\lambda]r^1\rho^2|[\lambda_1]r^1(\omega_0^1),[\lambda_2]r^2(\omega_0^2)\rangle$$
$$= \frac{N_1!N_2!f_\lambda}{N!f_{\lambda_1}f_{\lambda_2}}\langle\lambda]r^1r^2|[\lambda]r^1\rho^2\rangle\langle[\lambda]r^1\bar{\rho}^2|[\lambda]r^1\bar{r}^2\rangle. \tag{43}$$

This implies the following simple relationship between transformation and coupling coefficients (assuming from now on that a real representation of these coefficients is used):

$$\langle[\lambda_1]r^1(\omega_0^1),[\lambda_2]r^2(\omega_0^2)|[\lambda]r^1\rho^2\rangle = \gamma(\lambda_1,\lambda_2;\lambda)\langle[\lambda]r^1r^2|[\lambda]r^1\rho^2\rangle, \tag{44}$$

where the proportionality factor γ has the form (cf. also eq. (4-179a) of ref. [67])

$$\gamma(\lambda_1,\lambda_2;\lambda) = \left(\frac{N_1!N_2!f_\lambda}{N!f_{\lambda_1}f_{\lambda_2}}\right)^{1/2}. \tag{45}$$

Example

To conclude this section, we illustrate the above-introduced notation and definitions on a simple example, alluded to already in eqs. (8) and (9). Consider the symmetric group S_5 together with the chain $S_5 \supset S_3 \times S_2$. The standard basis for the five-dimensional irrep $[2^21]$ can thus be labeled in one of the following ways:

$$|[2^21]\,3,2,2,1,1\rangle = \left|\begin{matrix}1&2\\3&4\\5\end{matrix}\right\rangle = \left|[2^21]\begin{matrix}1&2&\cdot&4\\3&&5\end{matrix}\right\rangle, \tag{46a}$$

$$|[2^21]\,3,2,1,2,1\rangle = \left|\begin{matrix}1&3\\2&4\\5\end{matrix}\right\rangle = \left|[2^21]\begin{matrix}1&3&\cdot&4\\2&&5\end{matrix}\right\rangle, \tag{46b}$$

$$|[2^2 1]\,2,3,2,1,1\rangle = \left|\begin{matrix}1 & 2\\ 3 & 5\\ 4\end{matrix}\right\rangle = \left|[2^2 1]\begin{matrix}1 & 2 & \cdot & 5\\ 3 & & 4\end{matrix}\right\rangle, \tag{46c}$$

$$|[2^2 1]\,2,3,1,2,1\rangle = \left|\begin{matrix}1 & 3\\ 2 & 5\\ 4\end{matrix}\right\rangle = \left|[2^2 1]\begin{matrix}1 & 3 & \cdot & 5\\ 2 & & 4\end{matrix}\right\rangle, \tag{46d}$$

$$|[2^2 1]\,2,1,3,2,1\rangle = \left|\begin{matrix}1 & 4\\ 2 & 5\\ 3\end{matrix}\right\rangle = \left|\begin{matrix}\quad 1 & \\ [2^2 1]2 & 4\\ \quad 3 & 5\end{matrix}\right\rangle, \tag{46e}$$

where the first symbol uses a Yamanouchi symbol, the second one a Young tableau (that automatically implies the Young diagram $[2^2 1]$ which we thus omit) and, finally, the third symbol employs the $S_3 \times S_2$ subgroup tableau decomposition $r = r^1 \rho^2$. In contrast, the non-canonical basis vectors for the same irrep of S_5 based on the chain $S_5 \supset S_3 \times S_2$ are

$$\left|[2^2 1]\begin{matrix}1 & 2 & & 4 & 5\\ 3\end{matrix}\right\rangle, \tag{47a}$$

$$\left|[2^2 1]\begin{matrix}1 & 2 & 4\\ 3 & & 5\end{matrix}\right\rangle, \tag{47b}$$

$$\left|[2^2 1]\begin{matrix}1 & 3 & & 4 & 5\\ 2\end{matrix}\right\rangle, \tag{47c}$$

$$\left|[2^2 1]\begin{matrix}1 & 3 & 4\\ 2 & & 5\end{matrix}\right\rangle, \tag{47d}$$

$$\left|\begin{matrix}\quad 1 & \\ [2^2 1]\,2 & 4\\ \quad 3 & 5\end{matrix}\right\rangle, \tag{47e}$$

Obviously, the first two basis vectors (47a) and (47b) can be obtained as linear combinations of vectors (46a) and (46c) and, similarly, (47c) and (47d) as linear combinations of (46b) and (46d). The last vector (47e) corresponds directly to (46e). The transforma-

tion coefficients defined by eq. (34) obviously give the overlaps between canonical and non-canonical basis vectors (46) and (47), respectively.

Considering next outer products of S_3 and S_2 irreps, we easily find (using Littlewood rules) that the $[2^2 1]$ irrep of S_5 can be obtained in either of the following ways:

$$\begin{matrix}[2\ 1]\otimes[2] = [4\ 1] \oplus [3\ 2] \oplus [2^2 1] \oplus [3\ 1^2] \\ \quad (20) \qquad (4) \qquad (5) \qquad (5) \qquad (6)\ ,\end{matrix} \tag{48a}$$

$$\begin{matrix}[2\ 1]\otimes[1^2] = [2\ 1^3] \oplus [3\ 2] \oplus [2^2 1] \oplus [3\ 1^2] \\ \quad (20) \qquad (4) \qquad (5) \qquad (5) \qquad (6)\ ,\end{matrix} \tag{48b}$$

$$\begin{matrix}[1^3]\otimes[1^2] = [1^5] \oplus [2\ 1^3] \oplus [2^2 1] \\ \quad (10) \qquad (1) \qquad (4) \qquad (5)\ ,\end{matrix} \tag{48c}$$

where below each equation the numbers enclosed in parentheses indicate the relevant dimensions. The required S_5 basis vectors carrying $[2^2 1]$ can thus be obtained as linear combinations of product states of types $|[2\ 1]r\rangle|[2]s\rangle$, $|[2\ 1]r\rangle|[1^2]s\rangle$, or $|[1^3]r\rangle|[1^2]s\rangle$ using the outer product coupling coefficients defined by eq. (23).

2.3. S_N ISOSCALAR FACTORS

An important property of both coupling and transformation coefficients that are associated with bases adapted to canonical chains (3) or (6) is their factorization into the product of factors, which can be fully characterized by the irrep labels for pairs of neighbouring subgroups in the chain. These factors are referred to as *isoscalar factors* or *reduced Wigner coefficients* [55,71]. The subsequent paper of this series will show that they are closely related to the *segment values* of the UGA [6,8], and that they reveal the composite structure of canonical bases and related coupling and transformation coefficients.

We first turn our attention to the *outer product isoscalar factors* (I_o factors), which are defined as the ratio of two outer product coupling coefficients

$$I_o\begin{pmatrix}[\lambda_1] & [\lambda_2] & | & [\lambda] \\ [\mu_1] & [\mu_2] & | & [\mu]\end{pmatrix} \equiv \begin{pmatrix}[\lambda_1] & [\lambda_2] & | & [\lambda] \\ [\mu_1] & [\mu_2] & | & [\mu]\end{pmatrix}_o \equiv \begin{pmatrix}[\lambda_1] & [\lambda_2] & | & [\lambda] \\ [\mu_1] & [\mu_2] & | & [\mu]\end{pmatrix}$$

$$= \langle [\lambda_1]r^1(\omega^1), [\lambda_2]r^2(\omega^2)|[\lambda]r\rangle \cdot \langle [\mu_1]s^1(\omega'^1), [\mu_2]s^2(\omega'^2)|[\mu]s\rangle^{-1}, \tag{49}$$

where s results when we remove the box containing the label N from the Young tableau r, as schematically illustrated in fig. 1. Likewise, there are two possibilities for $[\mu_1]$ and $[\mu_2]$. If $N \in \omega_2$, then

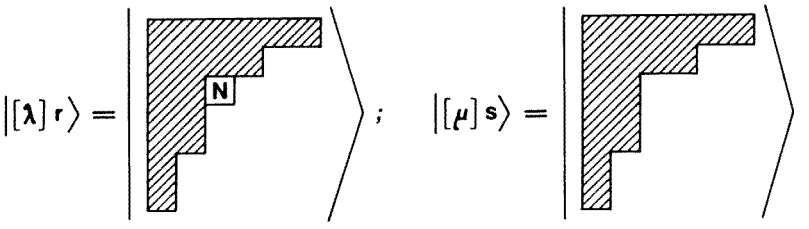


Fig. 1. Schematic representation of Young tableaux characterizing the Nth level isoscalar factor.

$$[\lambda_1] = [\mu_1] \quad \text{and} \quad |[\lambda_1] r^1(\omega^1)\rangle = |[\mu_1] s^1(\omega'^1)\rangle,$$

so that $s^2(\omega'^2)$ results from $r^2(\omega^2)$ by deleting the box containing N. If, on the other hand, $N \in \omega^1$, we have that

$$|[\lambda_2] r^2(\omega^2)\rangle = |[\mu_2] s^2(\omega'^2)\rangle$$

and $s^1(\omega'^1)$ results by deleting N in the tableau $r^1(\omega^1)$. Note that although we defined the isoscalar factor for the Nth level in order to keep our notation as simple as possible, this definition applies to any level in the canonical chain (3) or (6). Then, using the definition (49) recursively, we can express any outer product coupling coefficient as a product of isoscalar factors

$$\langle [\lambda_1] r^1(\omega^1), [\lambda_2] r^2(\omega^2) | [\lambda] r\rangle = \prod_{i=2}^{N} \begin{pmatrix} [\mu_1^{(i)}] & [\mu_2^{(i)}] & | & [\mu^{(i)}] \\ [\mu_1^{(i-1)}] & [\mu_2^{(i-1)}] & | & [\mu^{(i-1)}] \end{pmatrix}, \tag{50}$$

where $\mu_1^{(N)} \equiv \lambda_1$, $\mu_2^{(N)} \equiv \lambda_2$, $\mu^{(N)} = \lambda$, since the S_1 outer product coupling coefficients $\langle [1](1)[0](0) | [1](1)\rangle = \langle [0](0)[1](1) | [1](1)\rangle$, appearing in the last isoscalar factor, are equal to one.

We next consider the subduction $S_N \downarrow S_{N_1} \times S_{N_2}$ and define the *isoscalar factor* I_s (*subduction* isoscalar factor) for a nonstandard, partitioned basis (5) as

$$I_s \begin{pmatrix} [\lambda_1] & [\lambda_2] & | & [\lambda] \\ [\mu_1] & [\mu_2] & | & [\mu] \end{pmatrix} \equiv \begin{pmatrix} [\lambda_1] & [\lambda_2] & | & [\lambda] \\ & [\mu_2] & | & [\mu] \end{pmatrix}_s \equiv \begin{pmatrix} [\lambda_1] & [\lambda_2] & | & [\lambda] \\ & [\mu_2] & | & [\mu] \end{pmatrix}$$

$$= \langle [\lambda] r^1 r^2 | [\lambda] r^1 \rho^2\rangle \cdot \langle [\mu] r^1 r'^2 | [\mu] r^1 \rho'^2\rangle^{-1}. \tag{51}$$

We note that these factors are also sometimes referred to as the symmetric group reduced transformation coefficients (RTC) or reduced subduction coefficients (RSDC) [67]. Recall that $|[\lambda] r^1 r^2\rangle \equiv |[\lambda]; [\lambda_1] r^1, [\lambda_2] r^2\rangle$ with Young tableaux r^1 labeled by

$1, 2, \ldots, N_1$ and r^2 by $N_1 + 1, N_1 + 2, \ldots, N_1 + N_2 = N$, and $r^1\rho'^2$ and r'^2 resulting, respectively, from $r \equiv r^1\rho^2$ and r^2 by deleting the box labeled with N (or, equivalently, by dropping the first label in the corresponding Yamanouchi symbols). We see that in contrast to the I_o factor, the first irrep $[\lambda_1]$ is always the same in the I_s factor, so that it does not have to be repeated and enables us to graphically distinguish both factors. Should the danger of confusion arise, however, we shall employ the notation indicating I_o and I_s explicitly (or as a subscript). In any case, it is easily seen from eq. (44) that both factors are simply related, namely

$$I_o\begin{pmatrix}[\lambda_1] & [\lambda_2] & | & [\lambda]\\ [\mu_1] & [\mu_2] & | & [\mu]\end{pmatrix} = \frac{\gamma(\lambda_1, \lambda_2; \lambda)}{\gamma(\mu_1, \mu_2; \mu)} I_s\begin{pmatrix}[\lambda_1] & [\lambda_2] & | & [\lambda]\\ [\lambda_1] & [\mu_2] & | & [\mu]\end{pmatrix}. \tag{52}$$

Since, in fact, $[\lambda_1] = [\mu_1]$ for I_s, we have that

$$\begin{pmatrix}[\lambda_1] & [\lambda_2] & | & [\lambda]\\ & [\mu_2] & | & [\mu]\end{pmatrix} = \left[\frac{N f_{\lambda_2} f_\mu}{N_2 f_\lambda f_{\mu_2}}\right]^{1/2}\begin{pmatrix}[\lambda_1] & [\lambda_2] & | & [\lambda]\\ [\lambda_1] & [\mu_2] & | & [\mu]\end{pmatrix}. \tag{53}$$

3. U(n) isoscalar factors

We shall next consider irreps $\langle\lambda\rangle$ of U(n), where λ is again a partition of N with at most n components $\lambda_1, \lambda_2, \ldots, \lambda_n$, $\sum_i \lambda_i = N$, while N is arbitrary. The dimension d_λ of $\langle\lambda\rangle$ is given by the Weyl–Robinson formula [79–81] and the standard basis is that adapted to the Gel'fand–Tsetlin chain [25], which we write schematically as

$$\mathrm{U}(n) \supset \mathrm{U}(n-1) \supset \ldots \supset \mathrm{U}(2) \supset \mathrm{U}(1). \tag{54}$$

This basis can be labeled either by Gel'fand tableaux (m) or by Weyl tableaux W. For electronic Gel'fand–Tsetlin states, we can also use an efficient ABC (or Paldus) tableau or related step number labeling [1,6–8]. The relationship between these various labeling schemes is well known [7,8,82].

In general developments described in this work, we shall primarily employ Weyl tableau labeling for the following two reasons: (i) it facilitates the establishment and exploitation of the S_N–U(n) duality in view of a simple correspondence between Young and Weyl tableaux, and (ii) it makes the formulation independent of the order of the unitary group n. Consequently, our expressions for the U(n) CG coefficients, isoscalar factors, segment values, etc., will also be n-independent and, hence, applicable to any chain U(m) $\supset$ U($m-1$) or any orbital level in many-electron theory applications. This is clearly an important and beneficial feature of our formulation, since not only can n be fairly large when handling many-electron problems, but this also makes the formulas

independent of the orbital basis size. When we restrict our considerations to at most two-column tableaux that are relevant for many-electron systems, it is straightforward to recast the relevant formulas into the most convenient labeling scheme for a given problem, be it ABC tableaux or its various sub-tableaux, step number labeling, etc.

It is also useful to recall that the U(n) Clebsch–Gordan coefficients can be defined in two different ways: (i) either as the coupling coefficients for basis states (e.g. Gel'fand–Tsetlin basis), or (ii) as the matrix elements of Wigner operators (in which case it seems more appropriate to call them Wigner coefficients [46,53]). Clearly, our main objective is to calculate matrix elements of U(n) generators and products of such generators, through which one can express quantum mechanical operators associated with various observables of physical and chemical interest. This will be done not only for the canonical Gel'fand– Tsetlin basis, but also for bases which are suitable when considering a system partitioning [14,40,83]. Thus, our objective represents a special case of a more general problem of matrix element evaluation of general U(n) tensor operators, to which this series of papers is devoted. In contrast to existing methodology in this regard, we intend to exploit the close relationship between unitary and symmetric groups, as outlined in the introduction.

Designating Gel'fand–Tsetlin basis states for an irrep $\langle \nu \rangle$ by $\left| {\langle \nu \rangle \atop W} \right\rangle$, we define the U($n$) coupling coefficients as

$$\left| {\langle \nu \rangle \atop W} \right\rangle = \sum_{U,V} \left\langle {\langle \lambda \rangle \quad \langle \mu \rangle \atop U \quad V} \middle| {\langle \nu \rangle \atop W} \right\rangle_{\mathrm{u}} \left| {\langle \lambda \rangle \atop U} \right\rangle \left| {\langle \mu \rangle \atop V} \right\rangle , \tag{55}$$

where $\langle \lambda \rangle$, $\langle \mu \rangle$ and $\langle \nu \rangle$ are irreps of U(n) and U, V and W are corresponding Weyl tableaux, labeling basis vectors of their carrier spaces, respectively. Clearly, these coupling coefficients are nonvanishing only when $\langle \nu \rangle \subset \langle \lambda \rangle \otimes \langle \mu \rangle$. Moreover, we assume that each irrep $\langle \nu \rangle$ appears in the product $\langle \lambda \rangle \otimes \langle \mu \rangle$ at most once which is not, of course, the case in general when $\langle \nu \rangle$ can occur with nonunit multiplicity. In the general case, we thus require additional labels which resolve this multiplicity problem. However, in the actual applications which we have in mind, we deal with special irreps characterizing the many-electron systems. Since in these circumstances the multiplicity problem can be avoided in most cases, and we do not wish to make our notation unnecessarily cumbersome, we shall in the following assume that $\langle \nu \rangle$ occurs at most once in the direct product $\langle \lambda \rangle \otimes \langle \mu \rangle$.

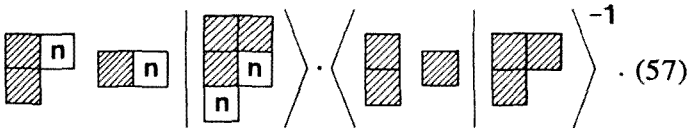
In complete analogy with the symmetric group, we then define the (nth level) U(n) isoscalar factor

$$I_{\mathrm{u}} \begin{pmatrix} \langle \lambda \rangle & \langle \mu \rangle & \langle \nu \rangle \\ \langle \lambda' \rangle & \langle \mu' \rangle & \langle \nu' \rangle \end{pmatrix} \equiv \begin{pmatrix} \langle \lambda \rangle & \langle \mu \rangle & \langle \nu \rangle \\ \langle \lambda' \rangle & \langle \mu' \rangle & \langle \nu' \rangle \end{pmatrix}_{\mathrm{u}} \equiv \begin{pmatrix} \langle \lambda \rangle & \langle \mu \rangle & \langle \nu \rangle \\ \langle \lambda' \rangle & \langle \mu' \rangle & \langle \nu' \rangle \end{pmatrix}$$

$$= \left\langle {\langle \lambda \rangle \quad \langle \mu \rangle \atop U \quad V} \middle| {\langle \nu \rangle \atop W} \right\rangle_{\mathrm{u}} \left\langle {\langle \lambda' \rangle \quad \langle \mu' \rangle \atop U' \quad V'} \middle| {\langle \nu' \rangle \atop W'} \right\rangle_{\mathrm{u}}^{-1} , \tag{56}$$

where $\langle\lambda'\rangle$, $\langle\mu'\rangle$ and $\langle\nu'\rangle$ are irreps of U($n-1$) and U', V' and W' are corresponding U($n-1$) Weyl tableaux that are obtained from U, V and W by deleting the boxes carrying the label n. Thus, for example,

$$\begin{pmatrix} \langle 2\,1\rangle & \langle 2\rangle \\ \langle 1^2\rangle & \langle 1\rangle \end{pmatrix} \left| \begin{matrix} \langle 2^2 1\rangle \\ \langle 2\,1\rangle \end{matrix} \right) =$$



(57)

Note that here and in the following text we drop the irrep labels when they are automatically implied by the explicit form of the Weyl tableau.

Similarly, as in the case of the symmetric group, we shall also consider bases that are adapted to the chain

$$\mathrm{U}(n) \supset \mathrm{U}(n_1) \times \mathrm{U}(n_2), \qquad n_1 + n_2 = n, \tag{58}$$

and that are suitable when considering a system partitioning [14,40,83]. Labeling the basis states adapted to this chain as (cf. eqs. (53,54) of ref. [14])

$$\left| \langle\lambda\rangle \quad \begin{matrix} \langle\lambda_1\rangle \\ W_1 \end{matrix} \quad \begin{matrix} \langle\lambda_2\rangle \\ W_2 \end{matrix} \right\rangle \equiv |\langle\lambda\rangle W_1 W_2\rangle$$

(we again avoid the multiplicity labels, which are not required for at most two-column irreps), we define the transformation coefficients by

$$\left| \langle\lambda\rangle \quad \begin{matrix} \langle\lambda_1\rangle \\ W_1 \end{matrix} \quad \begin{matrix} \langle\lambda_2\rangle \\ W_2 \end{matrix} \right\rangle = \sum_W \left\langle \begin{matrix} \langle\lambda\rangle \\ W \end{matrix} \middle| \begin{matrix} \langle\lambda_1\rangle \\ W_1 \end{matrix} \quad \begin{matrix} \langle\lambda_2\rangle \\ W_2 \end{matrix} \right\rangle_t \left| \begin{matrix} \langle\lambda\rangle \\ W \end{matrix} \right\rangle . \tag{59}$$

The U(n_1) and U(n_2) Weyl tableaux W_1 and W_2 involve, respectively, the labels $1, 2, \ldots, n_1$ and $n_1+1, n_1+2, \ldots, n_1+n_2 = n$. Since the partial Weyl tableau $\tilde{W}_1$, which is obtained when deleting boxes carrying labels greater than n_1 in the U(n) tableau W, so that we can write $\tilde{W}_1 = W \downarrow \mathrm{U}(n_1)$, must coincide with the U(n_1) tableau W_1, so that

$$\left\langle \begin{matrix} \langle\lambda_1\rangle \\ W_1 \end{matrix} \quad \begin{matrix} \langle\lambda_2\rangle \\ W_2 \end{matrix} \middle| \begin{matrix} \langle\lambda\rangle \\ W \end{matrix} \right\rangle_t = \delta_{W_1\tilde{W}_1} \left\langle \begin{matrix} \langle\lambda_1\rangle \\ W_1 \end{matrix} \quad \begin{matrix} \langle\lambda_2\rangle \\ W_2 \end{matrix} \middle| \begin{matrix} \langle\lambda\rangle \\ W \end{matrix} \right\rangle_t ,$$

$$\tilde{W}_1 = W \downarrow \mathrm{U}(n_1), \tag{60}$$

the sum in eq. (59) extends only over Weyl tableaux W with their $\tilde{W}_1$ part fixed. Consequently, the inverse transformation will involve only the summation over the U(n_2) labels, namely

$$\left|\begin{matrix}\langle\lambda\rangle\\ W\end{matrix}\right\rangle = \sum_{\langle\lambda_2\rangle, W_2} \left\langle\begin{matrix}\langle\lambda_1\rangle & \langle\lambda_2\rangle \\ W_1 & W_2\end{matrix}\middle|\begin{matrix}\langle\lambda\rangle\\ W\end{matrix}\right\rangle_t \left|\begin{matrix}\langle\lambda\rangle & \langle\lambda_1\rangle & \langle\lambda_2\rangle\\ & W_1 & W_2\end{matrix}\right\rangle. \tag{61}$$

We note the formal similarity of these $U(n) \downarrow U(n_1) \times U(n_2)$ transformation coefficients with the $U(n)$ CG coefficients (cf. eqs. (55) and (61)), which we distinguish by appropriate subscripts (at least when confusion could arise). These transformation coefficients can also be factored into a product of I_t (*transformation*) *isoscalar factors* (or $U(n)$ RTCs or RSDCs [67]), defined analogously as the I_u factors (eq. (56)) (cf. also definition (51))

$$I_t\begin{pmatrix}\langle\lambda_1\rangle & \langle\lambda_2\rangle \mid \langle\lambda\rangle\\ \langle\lambda_1\rangle & \langle\mu_2\rangle \mid \langle\mu\rangle\end{pmatrix} \equiv \begin{pmatrix}\langle\lambda_1\rangle & \langle\lambda_2\rangle \mid \langle\lambda\rangle\\ & \langle\mu_2\rangle \mid \langle\mu\rangle\end{pmatrix}_t \equiv \begin{pmatrix}\langle\lambda_1\rangle & \langle\lambda_2\rangle \mid \langle\lambda\rangle\\ & \langle\mu_2\rangle \mid \langle\mu\rangle\end{pmatrix}$$

$$= \left\langle\begin{matrix}\langle\lambda_1\rangle & \langle\lambda_2\rangle \\ W_1 & W_2\end{matrix}\middle|\begin{matrix}\langle\lambda\rangle\\ W\end{matrix}\right\rangle_t \left\langle\begin{matrix}\langle\lambda_1\rangle & \langle\mu_2\rangle \\ W_1 & W_2'\end{matrix}\middle|\begin{matrix}\langle\mu\rangle\\ W'\end{matrix}\right\rangle_t^{-1}, \tag{62}$$

where W_2' and W' result, respectively, from W_2 and W by a removal of boxes carrying the label n.

Thus, for each S_N or $U(n)$ coupling or transformation coefficient we can write a factorization formula similar to that given by eq. (50). The number of factors is given by N for the symmetric group (i.e. by an electron number in our applications) and by n in the case of $U(n)$ (i.e. by an orbital number). We shall see, however, that for problems which are relevant in applications, most of the factors in the $U(n)$ factorization have unit values and thus can be ignored.

In concluding our definitions, we briefly summarize the orthogonality properties of $U(n)$ CG and transformation coefficients, as well as of the corresponding isoscalar factors:

(i) *CG coefficients and I_u factors:*

$$\sum_{U,V} \left\langle\begin{matrix}\langle\nu\rangle\\ W\end{matrix}\middle|\begin{matrix}\langle\lambda\rangle & \langle\mu\rangle\\ U & V\end{matrix}\right\rangle_u \left\langle\begin{matrix}\langle\lambda\rangle & \langle\mu\rangle\\ U & V\end{matrix}\middle|\begin{matrix}\langle\nu'\rangle\\ W'\end{matrix}\right\rangle_u = \delta_{\nu\nu'}\delta_{WW'}, \tag{63}$$

$$\sum_{\nu,W} \left\langle\begin{matrix}\langle\lambda\rangle & \langle\mu\rangle\\ U & V\end{matrix}\middle|\begin{matrix}\langle\nu\rangle\\ W\end{matrix}\right\rangle_u \left\langle\begin{matrix}\langle\nu\rangle\\ W\end{matrix}\middle|\begin{matrix}\langle\lambda\rangle & \langle\mu\rangle\\ U' & V'\end{matrix}\right\rangle_u = \delta_{UU'}\delta_{VV'}, \tag{64}$$

$$\sum_{\lambda',\mu'} \begin{pmatrix}\langle\nu\rangle \mid \langle\lambda\rangle & \langle\mu\rangle\\ \langle\nu''\rangle \mid \langle\lambda'\rangle & \langle\mu'\rangle\end{pmatrix}\begin{pmatrix}\langle\lambda\rangle & \langle\mu\rangle \mid \langle\nu'\rangle\\ \langle\lambda'\rangle & \langle\mu'\rangle \mid \langle\nu''\rangle\end{pmatrix} = \delta_{\nu\nu'}, \tag{65}$$

$$\sum_{\nu}\begin{pmatrix}\langle\lambda\rangle & \langle\mu\rangle \\ \langle\lambda'\rangle & \langle\mu'\rangle\end{pmatrix}\begin{pmatrix}\langle\nu\rangle \\ \langle\nu'\rangle\end{pmatrix}\begin{pmatrix}\langle\nu\rangle \\ \langle\nu'\rangle\end{pmatrix}\begin{pmatrix}\langle\lambda\rangle & \langle\mu\rangle \\ \langle\lambda''\rangle & \langle\mu''\rangle\end{pmatrix} = \delta_{\lambda'\lambda''}\delta_{\mu'\mu''}; \tag{66}$$

(ii) *transformation coefficients and I_t factors:*

$$\sum_{\lambda_2,W_2}\left\langle\begin{matrix}\langle\lambda\rangle \\ W\end{matrix}\middle|\begin{matrix}\langle\lambda_1\rangle & \langle\lambda_2\rangle \\ W_1 & W_2\end{matrix}\right\rangle_t\left\langle\begin{matrix}\langle\lambda_1\rangle & \langle\lambda_2\rangle \\ W_1 & W_2\end{matrix}\middle|\begin{matrix}\langle\lambda'\rangle \\ W'\end{matrix}\right\rangle_t = \delta_{\lambda\lambda'}\delta_{WW'}, \tag{67}$$

$$\sum_{W}\left\langle\begin{matrix}\langle\lambda_1\rangle & \langle\lambda_2\rangle \\ W_1 & W_2\end{matrix}\middle|\begin{matrix}\langle\lambda\rangle \\ W\end{matrix}\right\rangle_t\left\langle\begin{matrix}\langle\lambda\rangle \\ W\end{matrix}\middle|\begin{matrix}\langle\lambda_1\rangle & \langle\lambda_2'\rangle \\ W_1 & W_2'\end{matrix}\right\rangle_t = \delta_{\lambda_2\lambda_2'}\delta_{W_2W_2'}, \tag{68}$$

$$\sum_{\lambda_2}\begin{pmatrix}\langle\lambda\rangle \\ \langle\mu\rangle\end{pmatrix}\begin{pmatrix}\langle\lambda_1\rangle & \langle\lambda_2\rangle \\ \langle\mu_2\rangle\end{pmatrix}\begin{pmatrix}\langle\lambda_1\rangle & \langle\lambda_2\rangle \\ \langle\mu_2\rangle\end{pmatrix}\begin{pmatrix}\langle\lambda\rangle \\ \langle\mu'\rangle\end{pmatrix} = \delta_{\mu\mu'}, \tag{69}$$

$$\sum_{\mu}\begin{pmatrix}\langle\lambda_1\rangle & \langle\lambda_2\rangle \\ \langle\mu_2\rangle\end{pmatrix}\begin{pmatrix}\langle\lambda\rangle \\ \langle\mu\rangle\end{pmatrix}\begin{pmatrix}\langle\lambda\rangle \\ \langle\mu\rangle\end{pmatrix}\begin{pmatrix}\langle\lambda_1\rangle & \langle\lambda_2'\rangle \\ \langle\mu_2\rangle\end{pmatrix} = \delta_{\lambda_2\lambda_2'}. \tag{70}$$

We stress again that for simplicity's sake we omit multiplicity indices in all the above expressions. General expressions can be found in ref. [74]. We also note the similarity between both sets of relations, eqs. (63) to (66) and (67) to (70). Note, however, that this similarity is only a formal one. Thus, for example, while we must sum over both Weyl tableaux in eq. (63) (note the parallel with the SU(2) or angular momentum CGs), only the second one is summed in eq. (67) alongside with the irrep label, however. This is easily realized considering an example analogous to that given at the end of section 2.2. Thus, taking $\langle\lambda\rangle = \langle 2^2 1\rangle$, $\langle\lambda_1\rangle = \langle 2\ 1\rangle$, we have to consider both $\langle\lambda_2\rangle = \langle 2\rangle$ and $\langle\lambda_2\rangle = \langle 1^2\rangle$.

4. Relationship between the S_N and U(n) isoscalar factors

4.1. RECIPROCITY BETWEEN THE S_N AND U(n) IRREPS

The reciprocity between the S_N and U(n) (or, generally, GL(n, C)) irreps, first discussed by Schur and fully explored by Weyl [80], implies that a complete decomposition of the Nth rank tensor power $(\mathcal{V}_n)^{\otimes N}$ (where $\mathcal{V}_n$ is a carrier space of the defining representation of U(n) [or GL(n, C) $\simeq$ GL($\mathcal{V}_n$)]) into the irreducible subspaces with respect to S_N yields simultaneously a complete decomposition with respect to U(n) and vice versa. Another aspect of this reciprocity manifests itself in the reduction of S_N outer products and U(n) Kronecker products of irreps, both given by the well-known Littlewood–Richardson rules.

Thus, when we construct an S_N adapted basis for a tensor product of N single-particle states from $\mathcal{V}_n$, $\mathcal{V}_n = \mathrm{Span}\{\phi_{i_k} \mid k = 1, \ldots, n\}$, we obtain simultaneously irrep bases for U(n). The S_N adaption may be conveniently achieved by projecting the $\mathcal{V}_n^{\otimes N}$ monomials $\Omega(\omega)$,

$$\Omega(\omega) = \phi_{i_1}(1)\phi_{i_2}(2)\ldots\phi_{i_N}(N), \tag{71}$$

$$\omega = \{i_1, i_2, \ldots, i_N\}, \quad i_1 \le i_2 \le \ldots \le i_N, \tag{72}$$

with Young orthogonal (or Young–Yamanouchi) units $o_{sr}^{[\lambda]}$ (eq. (38)),

$$o_{sr}^{[\lambda]} = \frac{f_\lambda}{N!} \sum_{P \in S_N} D^{[\lambda]}(P)_{sr} P. \tag{38}$$

This produces the S_N adapted bases $\{o_{sr}^{[\lambda]}\Omega(\omega) | s = 1, \ldots, f_\lambda\}$, with r,ω fixed, carrying the irrep $[\lambda]$ of S_N, while each set $\{o_{sr}^{[\lambda]}\Omega(\omega) | r = 1, \ldots, f_\lambda$; all ordered ω's$\}$, with s arbitrary but fixed, spans the carrier space for $\langle\lambda\rangle$ of U(n). Clearly, in the U(n) case, different Young tableaux s can produce the same Weyl tableau W (and thus the same basis state) when the orbital set ω contains multiple occupancies. However, taken as a set, we obtain a basis for $\langle\lambda\rangle$ of U(n) of dimension d_λ. Moreover,

$$\sum_\lambda f_\lambda d_\lambda = n^N. \tag{73}$$

Now, when all the $i_k \in \omega$, $k = 1, \ldots, N$, are *distinct*, the Young–Yamanouchi (YY) states obtained in this way are identical with corresponding U(n) Gel'fand–Tsetlin (GT) states when properly normalized, i.e.

$$\left|\begin{matrix}\langle\lambda\rangle \\ W\end{matrix}\right\rangle \equiv \left|\begin{matrix}\langle\lambda\rangle \\ W\end{matrix}\right\rangle_s \equiv \left|\begin{matrix}\langle\lambda\rangle & [\lambda] \\ W & s\end{matrix}\right\rangle = |[\lambda]r\rangle = \mathcal{N} o_{sr}^{[\lambda]}\Omega(\omega), \tag{74}$$

where the Weyl tableau W is obtained by replacing the indices $1, 2, \ldots, N$ of the Young tableau r by the orbital labels ω, i.e. by applying the map (18) or (20),

$$\begin{bmatrix}\omega_0 \\ \omega\end{bmatrix} : j \mapsto i_j, \quad j = 1, \ldots, N, \tag{75}$$

where now the domain $\omega \subset \{1, 2, \ldots, n\}$ and can contain repetitions. The projector $o_{sr}^{[\lambda]}$ acts on the electronic coordinates $1, 2, \ldots, N$, and its first Young tableau s is arbitrary, but fixed. As indicated in eq. (74), we can often drop this index (see example below). The normalization factor is easily evaluated as

$$\mathcal{N}^2\langle o_{sr}^{[\lambda]}\Omega(\omega)\,|\,o_{sr}^{[\lambda]}\Omega(\omega)\rangle = 1$$

$$= \mathcal{N}^2\frac{f_\lambda}{N!}\sum_{P\in S_N} D^{[\lambda]}(P)_{rr}\langle\Omega(\omega)\,|\,P\Omega(\omega)\rangle$$

$$= \mathcal{N}^2\frac{f_\lambda}{N!}, \tag{76}$$

since only the identity permutation $P = e$ will satisfy the requirement that $P\Omega(\omega) = \Omega(\omega)$ when all the orbitals constituting $\Omega(\omega)$ (eq. (71)) are distinct. We can simply write

$$\left|\begin{matrix}\langle\lambda\rangle\\ W\end{matrix}\right\rangle = (N!/f_\lambda)^{1/2}o_{sr}^{[\lambda]}\Omega(\omega), \tag{77}$$

since W uniquely determines r.

Now assume that the highest label in ω is f-times occupied, i.e. that

$$i_N = i_{N-1} = \ldots = i_{N-f+1} = m, \quad m \le n, \tag{78}$$

while the remaining labels are again distinct. We thus require an additional normalization factor, which we designate as $[N(\lambda, \rho^2)]^{-1}$, so that

$$\left|\begin{matrix}\langle\lambda\rangle\\ W\end{matrix}\right\rangle = [N(\lambda,\rho^2)]^{-1}|[\lambda]r^1\rho^2\rangle$$

$$= [N(\lambda,\rho^2)]^{-1}(N!/f_\lambda)^{1/2}o_{sr}^{[\lambda]}\Omega(\omega). \tag{79}$$

The Young tableau r now consists of two parts: an r^1 part labeled by indices $1, 2, \ldots, N-f$ and a ρ^2 part, labeled by the remaining labels $N-f+1, \ldots, N$. The Weyl tableau W is again obtained by applying the map (75) to r, which now assigns the same label m to the last f indices, i.e.

$$j \mapsto i_j, \ (j = 1, \ldots, N-f) \quad \text{and} \quad \omega_0^2 = \{N-f+1, \ldots, N\} \to m. \tag{80}$$

In other words, the f-times occupied label m will appear everywhere in the partial tableau designated by ρ^2 (cf. section 2.1). Thus, in this case, $f!$ (or less if ω_0^2 labels appear in the same row) distinct Young tableau $r \equiv (r^1\rho^2)$, with identical r^1 subtableau, yield the same Weyl tableau, as schematically shown in fig. 2.

Evaluating the normalization factor $N(\lambda, \rho^2)$ as in the singly occupied case (eq. (76)), we realize that the sum over S_N will now involve $f!$ permutations P which give $P\Omega(\omega) = \Omega(\omega)$. These permutations form a group $S_f(\omega_0^2)$, so that

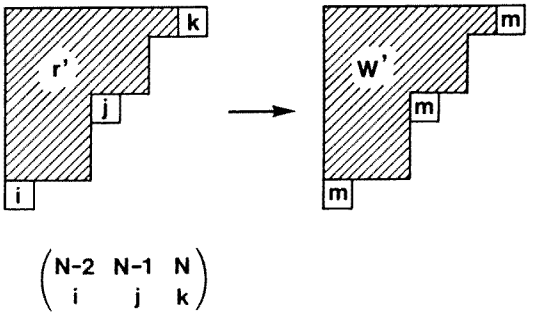


Fig. 2. Illustration of the Young tableaux yielding the same Weyl tableau when multiple occupancy f (e.g. $f = 3$) is present. The i, j, k can represent any of the $3! = 6$ permutations of $N-2$, $N-1$ and N.

$$N(\lambda,\rho^2)=\left[\sum_{P\in S_f(\omega_0^2)} D^{[\lambda]}(P)_{rr}\right]^{1/2}. \tag{81}$$

This relationship will hold even when S_f permutes another set of identical labels, not necessarily the highest ones. We note that a general analytical expression for this normalization factor can be found in ref. [84], eq. (5.9). Considering eq. (32) for $[\lambda_2] = [f]$, the totally symmetric representation of S_f, for which $D^{[f]}(P_2)_{\bar{r}^2,r^2} = \delta_{\bar{r}^2,r^2}$, we can also write for the normalization factor (81)

$$N(\lambda,\rho^2)=\left[\frac{N!f_{\lambda_1}}{(N-f)!f_\lambda}\right]^{1/2}\langle[\lambda_1]r^1[f](1)|[\lambda]r\rangle, \tag{82}$$

assuming that the outer product coupling coefficients are real. This coefficient can be expressed as a product of I_0 factors (eq. (50)). For greater notational compactness, we define multiple I_0 factors for this case as follows:

$$\begin{aligned}\langle[\lambda_1]r^1[f](1)|[\lambda]r\rangle &\equiv ([\lambda_1][f]|[\lambda])_r\\ &=\begin{pmatrix}[\lambda_1] & [f] & \\ [\lambda_1] & [f-1] & [\lambda-1(\rho^2)]\end{pmatrix}\begin{pmatrix}[\lambda_1] & [f-1] & \\ [\lambda_1] & [f-2] & [\lambda-2(\rho^2)]\end{pmatrix}\cdots\\ &\cdots\begin{pmatrix}[\lambda_1] & [1] & \\ [\lambda_1] & [0] & [\lambda_1]\end{pmatrix},\end{aligned} \tag{83}$$

where $[\lambda - k(\rho^2)]$ designates the irrep which results when k boxes with highest labels are removed from the Young tableau $r \equiv (r^1\rho^2)$ that is associated with irrep $[\lambda]$, so that

$$[\lambda - f(\rho^2)] = [\lambda_1]. \tag{84}$$

The considered case, eq. (78), applies generally, since restricting U(m) to U($m-1$) we obtain a valid relationship between YY and GT states. In the general case, we can thus proceed with multiple occupancies from the lowest multiple occupied level to the highest one, applying the normalization factor (81) or (82) at each stage.

Example:

Let us illustrate these developments on a simple example involving S_3 and U(n), $n = 2, 3, \ldots$. The only non-trivial Young orthogonal units are those associated with the two-dimensional irrep [2,1], in which case

$$\left.\begin{matrix} o_{11}^{[2,1]} \\ o_{22}^{[2,1]} \end{matrix}\right\} = \tfrac{1}{6}[2e \pm 2(12) \mp (13) \mp (23) - (123) - (132)], \tag{85a}$$

$$\left.\begin{matrix} o_{12}^{[2,1]} \\ o_{21}^{[2,1]} \end{matrix}\right\} = \tfrac{\sqrt{3}}{6}[(23) - (13) \pm (123) \mp (132)]. \tag{85b}$$

Choosing $\omega = \omega_0 = \{1,2,3\}$, we immediately obtain two distinct realizations of 3-electron states with unit occupancies (so that $n \geq 3$), namely

$$\left|\begin{matrix} 1 & 2 \\ 3 & \end{matrix}\right\rangle_1 \equiv \left|\begin{matrix} 1 & 2 & 1 & 2 \\ 3 & , & 3 & \end{matrix}\right\rangle = \sqrt{3}\, o_{11}^{[2,1]} \Omega(\omega_0) = \phi_+, \tag{86a}$$

$$\left|\begin{matrix} 1 & 3 \\ 2 & \end{matrix}\right\rangle_1 \equiv \left|\begin{matrix} 1 & 3 & 1 & 2 \\ 2 & , & 3 & \end{matrix}\right\rangle = \sqrt{3}\, o_{12}^{[2,1]} \Omega(\omega_0) = \psi_+, \tag{86b}$$

$$\left|\begin{matrix} 1 & 2 \\ 3 & \end{matrix}\right\rangle_2 \equiv \left|\begin{matrix} 1 & 2 & 1 & 3 \\ 3 & , & 2 & \end{matrix}\right\rangle = \sqrt{3}\, o_{21}^{[2,1]} \Omega(\omega_0) = \psi_-, \tag{86c}$$

$$\left|\begin{matrix} 1 & 3 \\ 2 & \end{matrix}\right\rangle_2 \equiv \left|\begin{matrix} 1 & 3 & 1 & 3 \\ 2 & , & 2 & \end{matrix}\right\rangle = \sqrt{3}\, o_{22}^{[2,1]} \Omega(\omega_0) = \phi_-, \tag{86d}$$

where

$$\phi_\pm = \tfrac{\sqrt{3}}{6}[2/123/ \pm 2/213/ \mp /321/ \mp /132/ - /312/ - /231/], \tag{87a}$$

$$\psi_\pm = \tfrac{1}{2}[/132/ - /321/ \pm /312/ \mp /231/], \tag{87b}$$

and where we defined

$$/i_1 i_2 i_3/ \equiv \phi_{i_1}(1)\phi_{i_2}(2)\phi_{i_3}(3). \tag{88}$$

When double occupancy is present, i.e. $\omega = \{1,2,2\}$, we find similarly

$$o_{1r}^{[2,1]}\Omega(\omega) = N_r\Phi, \qquad r = 1,2\,, \tag{89a}$$

$$o_{2r}^{[2,1]}\Omega(\omega) = M_r\Psi, \qquad r = 1,2\,, \tag{89b}$$

with

$$\Phi = /122/ + /212/ - 2/221/, \tag{90a}$$

$$\Psi = /122/ - /212/, \tag{90b}$$

and

$$N_1 = \tfrac{1}{6}, \quad N_2 = M_1 = \frac{\sqrt{3}}{6}, \quad M_2 = \tfrac{1}{2}\,. \tag{91}$$

Now, for any doubly occupied level, we easily find the normalization factor $N(\lambda,\rho^2)$ using eq. (81), namely

$$N(\lambda,\rho^2) = (1 + d_{N,N-1}^{-1})^{1/2}, \tag{92}$$

where d_{ij} is the axial distance from i to j in the standard Young tableau r. Thus, in the present case, for $r = (1) = \begin{smallmatrix}1&2\\3\end{smallmatrix}$, we have $d_{32} = -2$ and for $r = (2) = \begin{smallmatrix}1&3\\2\end{smallmatrix}$, $d_{32} = 2$, so that

$$N\left([2,1], \begin{matrix}\cdot & 2\\ 3 & \end{matrix}\right) \equiv n_1 = 1/\sqrt{2}, \tag{93a}$$

and

$$N\left([2,1], \begin{matrix}\cdot & 3\\ 2 & \end{matrix}\right) \equiv n_2 = \sqrt{3/2}. \tag{93b}$$

Thus, altogether

$$\left|\begin{matrix}1 & 2\\ 2 & \end{matrix}\right\rangle_1 = N(\lambda,\rho^2)^{-1}(3!/2)^{1/2}o_{1r}^{[2,1]}\Omega(\omega) = n_r^{-1}\sqrt{3}N_r\Phi = 6^{-1/2}\Phi, \tag{94a}$$

and

$$\left|\begin{matrix}1 & 2\\ 2 & \end{matrix}\right\rangle_2 = N(\lambda,\rho^2)^{-1}(3!/2)^{1/2}o_{2r}^{[2,1]}\Omega(\omega) = n_r^{-1}\sqrt{3}M_r\Psi = 2^{-1/2}\Psi, \tag{94b}$$

where again

$$\left|\begin{matrix}1 & 2\\ 2\end{matrix}\right\rangle_s \equiv \left|\begin{matrix}1 & 2\\ 2\end{matrix}\quad s\right\rangle \equiv \left|\begin{matrix}\langle 2,1\rangle & [2,\ 1]\\ 1\ 2 & \\ 2 & s\end{matrix}\right\rangle, \tag{95}$$

since the irreps $\langle 2,1\rangle$ and $[2,1]$ are automatically implied by the explicit form of the Weyl and Young tableaux, respectively. We see that the resulting GT states, both labeled with the same Weyl tableau $\begin{smallmatrix}1 & 2\\ 2\end{smallmatrix}$, are distinct and should be distinguished by the Young tableau s (eq. (95)).

Likewise, when $\omega = \{1,1,2\}$, we find similarly

$$\left|\begin{matrix}1 & 1\\ 2\end{matrix}\right\rangle_1 = 6^{-1/2}[2/112/ - /211/ - /121/], \tag{96a}$$

$$\left|\begin{matrix}1 & 1\\ 2\end{matrix}\right\rangle_2 = 2^{-1/2}[/121/ - /211/], \tag{96b}$$

although in this case the second tableau projectors $o_{s,2}^{[2,1]}$ produce a vanishing result (since doubly occupied labels would occur in the same column). The double occupancy normalization factor (92) now equals $\sqrt{2}$.

Thus, when we deal with a two-dimensional irrep $[2,1]$ of S_3, we can always find two distinct realizations of the corresponding U(n) basis. We should thus label the resulting GT states with both Weyl and Young tableaux, as indicated in eq. (95). However, since the U(n) irrep matrices are independent of the realization used, as given by the Young tableau s, we can omit this label as long as we always keep it fixed when evaluating the matrix elements. Indeed, we easily find, using the following representation of U(n) generators,

$$E_{ij} = \sum_{k=1}^{N} e_{ij}(k) = \sum_{k=1}^{N} |\phi_i(k)\rangle\langle\phi_j(k)|, \tag{97}$$

that, e.g.

$$2^{1/2}E_{23}\left|\begin{matrix}1 & 2\\ 3\end{matrix}\right\rangle_s = (2/3)^{1/2}E_{23}\left|\begin{matrix}1 & 3\\ 2\end{matrix}\right\rangle_s = \left|\begin{matrix}1 & 2\\ 2\end{matrix}\right\rangle_s, \tag{98a}$$

or

$$E_{12}\left|\begin{matrix}1 & 2\\ 2\end{matrix}\right\rangle_s = \left|\begin{matrix}1 & 1\\ 2\end{matrix}\right\rangle_s, \tag{98b}$$

independently of the label s. It is easy to verify that this result is in complete agreement with the corresponding U(n) result (e.g. the example given in ref. [5], figs. 1 and 26), e.g. for $n = 3$,

$$\left\langle \begin{matrix} 2\ 1\ 0 \\ 2\ 1 \\ 1 \end{matrix} \middle| E_{23} \middle| \begin{matrix} 2\ 1\ 0 \\ 2\ 0 \\ 1 \end{matrix} \right\rangle = 2^{-1/2}, \tag{99a}$$

$$\left\langle \begin{matrix} 2\ 1\ 0 \\ 2\ 1 \\ 1 \end{matrix} \middle| E_{23} \middle| \begin{matrix} 2\ 1\ 0 \\ 1\ 1 \\ 1 \end{matrix} \right\rangle = \left(\frac{3}{2}\right)^{1/2}, \tag{99b}$$

and

$$\left\langle \begin{matrix} 2\ 1\ 0 \\ 2\ 1 \\ 2 \end{matrix} \middle| E_{12} \middle| \begin{matrix} 2\ 1\ 0 \\ 2\ 1 \\ 1 \end{matrix} \right\rangle = 1, \tag{99c}$$

where the Gel'fand tableau notation has been used.

This example indicates that indeed the above given considerations apply generally, even though we considered explicitly only the case when the highest level is multiply occupied (for the general case, see [72,74] and references therein). In fact, the simple case considered above is entirely satisfactory for our purposes, since we shall be working with U(n) isoscalar factors, which are given by the ratio of U(n) and U($n-1$) CG coefficients and depend only on U(n) and U($n-1$) irrep labels. In particular, they are independent of the structure of the U($n-1$) states involved, so that we can conveniently choose the states with all the orbitals singly occupied (i.e. the so-called special GT states). Based on the S_N–U(n) reciprocity, we can interrelate the I_o factors for S_N with corresponding I_u factors for U(n), as has been shown in [74]. For the sake of completeness and simplicity, we now present the required form of this relationship.

4.2. RELATIONSHIP BETWEEN THE I_o AND I_u FACTORS

To find the relationship between the I_o and I_u factors, we first exploit the reciprocity between the S_N and U(n) irrep bases (eq. (79)). Writing eq. (23′) in the form

$$|[\lambda]r(\omega^1)\rangle|[\mu]s(\omega^2)\rangle = \sum_{[\nu]t^1\tau^2} \langle [\nu]t^1\tau^2|[\lambda]r(\omega^1)[\mu]s(\omega^2)\rangle|[\nu]t^1\tau^2\rangle, \tag{23′}$$

and replacing the S_N states by the U(n) states using eq. (79), we can write

$$\left|\begin{matrix}\langle\lambda\rangle \\ U\end{matrix}\right\rangle \left|\begin{matrix}\langle\mu\rangle \\ V\end{matrix}\right\rangle = \sum_{[\nu]t^1\tau^2} \frac{N(\nu,\tau^2)}{N(\lambda,\rho^2)N(\mu,\sigma^2)} \langle [\nu]t^1\tau^2 \,|\, [\lambda]r(\omega^1)[\mu]s(\omega^2)\rangle \left|\begin{matrix}\langle\nu\rangle \\ W\end{matrix}\right\rangle . \tag{55′}$$

Comparison with the reciprocal relation to eq. (55) shows that (cf. also eq. (7-146a) of ref. [67])

$$\left\langle \begin{matrix} \langle\lambda\rangle & \langle\mu\rangle \\ U & V \end{matrix} \middle| \begin{matrix} \langle\nu\rangle \\ W \end{matrix} \right\rangle_u = \sum_{\tau^2} \frac{N(\nu,\tau^2)}{N(\lambda,\rho^2)N(\mu,\sigma^2)} \langle [\lambda] r(\omega^1)[\mu] s(\omega^2) \,|\, [\nu] t^1 \tau^2 \rangle, \quad (100)$$

the sum extending over all r^2 tableaux which yield the same multiply occupied part of the Weyl tableau when the map (80) is carried out as illustrated in fig. 2. Thus, when only singly occupied orbitals occur, all $N(\lambda,\rho^2)$ factors equal one and we can identify U(n) and S_N coupling coefficients (eq. (100)). Expressing then the coupling coefficients in eq. (100) through isoscalar factors and U($n-1$) or S_{N-f} coefficients (eqs. (56) and (49), respectively) and assuming that the multiple occupancy occurs only at the highest levels so that U($n-1$) and S_{N-f} coefficients will cancel out, we find that

$$\begin{pmatrix} \langle\lambda\rangle & \langle\mu\rangle \\ \langle\lambda_1\rangle & \langle\mu_1\rangle \end{pmatrix} \begin{vmatrix} \langle\nu\rangle \\ \langle\nu_1\rangle \end{vmatrix} = \sum_{\tau^2} \frac{N(\nu,\tau^2)}{N(\lambda,\rho^2)N(\mu,\sigma^2)} \times \begin{pmatrix} \langle\lambda\rangle & [\mu] \\ [\lambda - f_1(\rho^2)] & [\mu - f_2(\sigma^2)] \end{pmatrix} \begin{vmatrix} [\nu] \\ [\nu - f(\tau^2)] \end{vmatrix}, \quad (101)$$

where the composite I_o factor on the right-hand side is defined similarly as in eq. (83) and involves f factors corresponding to sequential reduction from S_N to S_{N-f}. Clearly, analogously to eq. (84), $[\lambda_1] \equiv [\lambda - f_1(\rho^2)]$, $[\mu_1] \equiv [\mu - f_2(\sigma^2)]$ and $[\nu_1] \equiv [\nu - f(\tau^2)]$. The sum over τ^2 involves $f!$ terms associated with Young tableaux yielding the same Weyl tableau as illustrated in fig. 2.

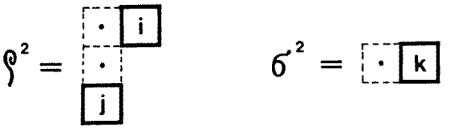
We note that we could also have started with the inverse relationship, eq. (23), rather than with eq. (23′) as we did. This would result in analogous expressions to those given in eqs. (100) and (101), which are sometimes preferable to use. Thus, in lieu of eq. (100), we would obtain (cf. also eq. (7-95) of ref. [67]):

$$\left\langle \begin{matrix} \langle\lambda\rangle & \langle\mu\rangle \\ U & V \end{matrix} \middle| \begin{matrix} \langle\nu\rangle \\ W \end{matrix} \right\rangle_u = \sum_{\omega^1,\omega^2} \sum_{\rho^2,\sigma^2} \frac{N(\lambda,\rho^2)N(\mu,\sigma^2)}{N(\nu,\tau^2)} \langle [\lambda] r(\omega^1)[\mu] s(\omega^2) | [\nu] t^1 \tau^2 \rangle, \quad (100')$$

and, likewise, for the isoscalar factors we find similarly to eq. (101)

$$\begin{pmatrix} \langle\lambda\rangle & \langle\mu\rangle \\ \langle\lambda_1\rangle & \langle\mu_1\rangle \end{pmatrix} \begin{vmatrix} \langle\nu\rangle \\ \langle\nu_1\rangle \end{vmatrix} = \sum_{\rho^2,\sigma^2} \frac{N(\lambda,\rho^2)N(\mu,\sigma^2)}{N(\nu,\tau^2)} \times \begin{pmatrix} [\lambda] & [\mu] \\ [\lambda - f_1(\rho^2)] & [\mu - f_2(\sigma^2)] \end{pmatrix} \begin{vmatrix} [\nu] \\ [\nu - f(\tau^2)] \end{vmatrix}, \quad (101')$$

Here, the sum over $\rho^2 \equiv \rho^2(\tilde{\omega})$ and $\sigma^2 \equiv \sigma^2(\tilde{\theta})$ must extend over all subtableaux ρ^2 and σ^2 with all possible orbital labelings $\tilde{\omega}$ and $\tilde{\theta}$, where $\{\tilde{\omega}, \tilde{\theta}\}$ consists of f labels being removed. For example, considering the isoscalar factor with $\langle\lambda\rangle = \langle 2\ 1^2\rangle$, $\langle\mu\rangle = \langle 2\rangle$ and $\langle\nu\rangle = \langle 3\ 2\ 1\rangle$ and $\langle\lambda_1\rangle = \langle 1^2\rangle$, $\langle\mu_1\rangle = \langle 1\rangle$, $\langle\nu_1\rangle = \langle 2\ 1\rangle$, so that $f_1 = 2, f_2 = 1$ and $f = 3$, the sum in eq. (101′) will involve 3! = 6 terms over the following subtableaux ρ^2, σ^2, shown in fig. 3. (Note that we need at least a three-column irrep $\langle\nu\rangle$ in order to obtain a non-vanishing result when $f = 3$.)



i	j	k
4	5	6
5	4	6
4	6	5
6	4	5
5	6	4
6	5	4

Fig. 3. An example that schematically illustrates the subtableaux that are involved in the sum in eq. (101′). See the text for details.

For many-electron systems, where at most double occupancies can occur, the summation in eq. (101) will involve at most two terms, and we present explicit expressions for all the possible cases below. Since we can encounter at most two-column irreps in this case, we introduce simplified explicit notation for the irreps, designating

$$[\lambda] = [2^a 1^b] =: (a, b),$$

$$[\mu] = [2^d 1^e] =: (d, e), \tag{102}$$

$$[\nu] = [2^s 1^t] =: (s, t),$$

where, clearly, $2(a + d) + b + e = 2s + t$, and similarly for the U(n) irreps (to distinguish I_u and I_o factors, we include corresponding subscripts). We thus have the following possibilities:

(i) when ϕ_n *is unoccupied*, both I_u and I_o factors equal one;

(ii) when ϕ_n *is singly occupied*, the I_u and I_o factors are identical, i.e.

$$\begin{pmatrix} (a,b) & (d,e) \\ (a',b') & (d',e') \end{pmatrix} \begin{vmatrix} (s,t) \\ (s',t') \end{vmatrix}_u = \begin{pmatrix} (a,b) & (d,e) \\ (a',b') & (d',e') \end{pmatrix} \begin{vmatrix} (s,t) \\ (s',t') \end{vmatrix}_o , \tag{103}$$

and the following possibilities can occur:

(a) $(a',b') = (a,b)$; $(d',e') = (d-1,e+1)$ or $(d,e-1)$ and $(s',t') = (s-1,t+1)$ or $(s,t-1)$;

(b) $(a',b') = (a-1,b+1)$ or $(a,b-1)$; $(d',e') = (d,e)$ and $(s',t') = (s-1,t+1)$ or $(s,t-1)$;

(iii) when ϕ_n *is doubly occupied*, the following cases must be distinguished:

(iiia) $f = 2$ *and* $f_1 = f_2 = 1$, i.e. we remove two boxes from ν and one box from each λ and μ. Using the normalization factor as given by eq. (92), we can write generally

$$\begin{pmatrix} \langle\lambda\rangle & \langle\mu\rangle \\ \langle\lambda-\Delta(\rho)\rangle & \langle\mu-\Delta(\sigma)\rangle \end{pmatrix} \begin{vmatrix} \langle\nu\rangle \\ \langle\nu-\Delta(\Gamma)\rangle \end{vmatrix} = \sum_{\tau^2} (1 + d^{-1}_{N,N-1}(\tau))^{1/2} \times \begin{pmatrix} [\lambda] & [\mu] \\ [\lambda-1(i)] & [\mu-1(j)] \end{pmatrix} \begin{vmatrix} [\nu] \\ [\nu-2(\tau^2)] \end{vmatrix}, \tag{104}$$

where

$$\Delta(\rho) = (0 \ldots 0\ 1\ 0 \ldots 0),$$

with 1 in the ρth place (i.e. removing a box from the ρth row), $\Delta(\Gamma) = \Delta(\gamma_1) + \Delta(\gamma_2)$, where γ_1 and γ_2 are the rows in which a box is removed in the irrep $\langle\nu\rangle$, and the sum extends over two possibilities, given by the order in which these boxes are removed. Explicitly, we obtain

$$\begin{pmatrix} (a,b) & (d,e) \\ (a',b') & (d',e') \end{pmatrix} \begin{vmatrix} (s,t) \\ (s-1,t) \end{vmatrix}_u = \left(\frac{t+2}{t+1}\right)^{1/2} \begin{pmatrix} (a,b) & (d,e) \\ (a',b') & (d,e) \end{pmatrix} \begin{vmatrix} (s,t) \\ (s-1,t+1) \end{vmatrix}$$

$$\times \begin{pmatrix} (a',b') & (d,e) \\ (a',b') & (d',e') \end{pmatrix} \begin{vmatrix} (s-1,t+1) \\ (s-1,t) \end{vmatrix}_o \tag{105}$$

$$+ \left(\frac{t}{t+1}\right)^{1/2} \begin{pmatrix} (a,b) & (d,e) \\ (a',b') & (d,e) \end{pmatrix} \begin{vmatrix} (s,t) \\ (s,t-1) \end{vmatrix}_o \begin{pmatrix} (a',b') & (d,e) \\ (a',b') & (d',e') \end{pmatrix} \begin{vmatrix} (s,t-1) \\ (s-1,t) \end{vmatrix}_o ,$$

where $(a',b') = (a-1,b+1)$ or $(a,b-1)$ and, similarly $(d',e') = (d-1,e+1)$ or $(d,e-1)$, and assuming that the label N occurs in λ and the label $(N-1)$ in μ. An equivalent but distinct formula results when N occurs in μ and $(N-1)$ in λ, namely

$$\begin{pmatrix} (a,b) & (d,e) \\ (a',b') & (d',e') \end{pmatrix} \begin{vmatrix} (s,t) \\ (s-1,t) \end{pmatrix}_u = \left(\frac{t+2}{t+1}\right)^{1/2} \begin{pmatrix} (a,b) & (d,e) \\ (a,b) & (d',e') \end{pmatrix} \begin{vmatrix} (s,t) \\ (s-1,t+1) \end{pmatrix}_o$$
$$\times \begin{pmatrix} (a,b) & (d',e') \\ (a',b') & (d',e') \end{pmatrix} \begin{vmatrix} (s-1,t+1) \\ (s-1,t) \end{pmatrix}_o \tag{106}$$
$$+ \left(\frac{t}{t+1}\right)^{1/2} \begin{pmatrix} (a,b) & (d,e) \\ (a,b) & (d',e') \end{pmatrix} \begin{vmatrix} (s,t) \\ (s,t-1) \end{pmatrix}_o \begin{pmatrix} (a,b) & (d',e') \\ (a',b') & (d',e') \end{pmatrix} \begin{vmatrix} (s,t-1) \\ (s-1,t) \end{pmatrix}_o .$$

(iiib) $f = 2, f_1 = 0, f_2 = 2$ (*or* $f_1 = 2, f_2 = 0$); i.e. both boxes are removed from tableaux ν and μ (or λ). Generally, we obtain

$$\begin{pmatrix} \langle\lambda\rangle & \langle\mu\rangle \\ \langle\lambda\rangle & \langle\mu-\Delta(\Sigma)\rangle \end{pmatrix} \begin{vmatrix} \langle\nu\rangle \\ \langle\nu-\Delta(\Gamma)\rangle \end{pmatrix} = \left(1+d^{-1}_{N,N-1}(\sigma)\right)^{-1/2} \sum_{\tau^2} \left(1+d^{-1}_{N,N-1}(\tau)\right)^{1/2}$$
$$\times \begin{pmatrix} [\lambda] & [\mu] \\ [\lambda] & [\mu-2(\sigma^2)] \end{pmatrix} \begin{vmatrix} [\nu] \\ [\nu-2(\tau^2)] \end{pmatrix}, \tag{107}$$

so that

$$\begin{pmatrix} (a,b) & (d,e) \\ (a,b) & (d-1,e) \end{pmatrix} \begin{vmatrix} (s,t) \\ (s-1,t) \end{pmatrix}_u$$
$$= \left(\frac{e+1}{e}\right)^{1/2} \left[\left(\frac{t+2}{t+1}\right)^{1/2} \begin{pmatrix} (a,b) & (d,e) \\ (a,b) & (d,e-1) \end{pmatrix} \begin{vmatrix} (s,t) \\ (s-1,t+1) \end{pmatrix}_o \right. \tag{108}$$
$$\times \begin{pmatrix} (a,b) & (d,e-1) \\ (a,b) & (d-1,e) \end{pmatrix} \begin{vmatrix} (s-1,t+1) \\ (s-1,t) \end{pmatrix}_o$$
$$\left. + \left(\frac{t}{t+1}\right)^{1/2} \begin{pmatrix} (a,b) & (d,e) \\ (a,b) & (d,e-1) \end{pmatrix} \begin{vmatrix} (s,t) \\ (s,t-1) \end{pmatrix}_o \begin{pmatrix} (a,b) & (d,e-1) \\ (a,b) & (d-1,e) \end{pmatrix} \begin{vmatrix} (s,t-1) \\ (s-1,t) \end{pmatrix}_o \right],$$

assuming that N occurs in the first column and $(N-1)$ in the second column in the Young tableau s of $[\mu]$ (i.e. in σ^2), or, equivalently

$$\begin{pmatrix}(a,b) & (d,e)\\(a,b) & (d-1,e)\end{pmatrix}\begin{vmatrix}(s,t)\\(s-1,t)\end{pmatrix}_{\mathrm{u}}=\left(\frac{e+1}{e+2}\right)^{1/2}\Bigg[\left(\frac{t+2}{t+1}\right)^{1/2}$$

$$\times\begin{pmatrix}(a,b) & (d,e)\\(a,b) & (d-1,e+1)\end{pmatrix}\begin{vmatrix}(s,t)\\(s-1,t+1)\end{pmatrix}_{\mathrm{o}}\begin{pmatrix}(a,b) & (d-1,e+1)\\(a,b) & (d-1,e)\end{pmatrix}\begin{vmatrix}(s-1,t+1)\\(s-1,t)\end{pmatrix}_{\mathrm{o}}$$

$$+\left(\frac{t}{t+1}\right)^{1/2}\begin{pmatrix}(a,b) & (d,e)\\(a,b) & (d-1,e+1)\end{pmatrix}\begin{vmatrix}(s,t)\\(s,t-1)\end{pmatrix}_{\mathrm{o}}\begin{pmatrix}(a,b) & (d-1,e+1)\\(a,b) & (d-1,e)\end{pmatrix}\begin{vmatrix}(s,t)\\(s-1,t)\end{pmatrix}_{\mathrm{o}}\Bigg], \tag{109}$$

when N occurs in the second and $(N-1)$ in the first column of the Young tableau s.

When $f_1 = 2$ and $f_2 = 0$, analogous formulas result, which can also be obtained using the symmetry property for the isoscalar factors; therefore, we do not present them here.

4.3. RELATIONSHIP BETWEEN THE I_s AND I_t FACTORS

Let us finally consider the relationship between the I_s factors for S_N and the I_t factors for U(n), which is completely analogous to the relationship (101).

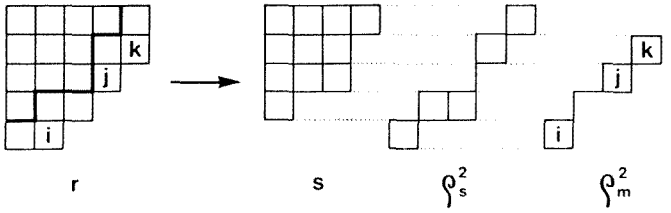
Starting again with the relationship (35),

$$|[\lambda];[\lambda_1]s,[\lambda_2]t\rangle=\sum_{\rho^2}\langle[\lambda]s\rho^2|[\lambda]st\rangle|[\lambda]s\rho^2\rangle, \tag{35}$$

and the corresponding one (eq. (59)) for the U(n), we assume that all the orbitals associated with W_1 are singly occupied while W_2 will have the highest label multiply occupied, so that we can make the corresponding tableau partitions, i.e. $t = t^1\tau^2$ and $\rho^2 = \rho_s^2\rho_m^2$ (note that $r = s\rho^2$), ρ_s^2, ρ_m^2 designating the singly and multiply occupied parts of ρ^2, as schematically shown in fig. 4. Using now the reciprocity relationship (eq. (79)) and comparing with eq. (59), we find that

$$\left\langle\begin{matrix}\langle\lambda\rangle\\W\end{matrix}\middle|\begin{matrix}\langle\lambda_1\rangle & \langle\lambda_2\rangle\\W_1 & W_2\end{matrix}\right\rangle_{\mathrm{t}}=\sum_{\rho_m^2}\frac{N(\lambda,\rho_m^2)}{N(\lambda_2,\tau^2)}\langle[\lambda]s\rho^2|[\lambda]st\rangle. \tag{110}$$

Clearly, the Weyl tableaux W_1, W_2 and W correspond to Young tableaux s, t and $r \equiv s\rho^2$, whose structure is schematically shown in fig. 4. Expressing the transformation coefficients in terms of corresponding isoscalar factors and U($m-1$) or S_{N-f} coefficients, which must be identical in view of the assumptions made above (since $N(\lambda,\rho^2) = 1$ in eq. (79) when only singly occupied orbitals are present), we obtain that



$$\begin{pmatrix} N-2 & N-1 & N \\ i & j & k \end{pmatrix} \quad \text{and} \quad \{i, j, k\} \longrightarrow m$$

Fig. 4. A schematic illustration of the partitioning of the Young tableau $r \equiv s\rho^2 \equiv s\rho_s^2\rho_m^2$, where $\{i,j,k\}$ represent a permutation of $\{N-2, N-1, N\}$ and are mapped onto the same orbital m when going to a corresponding Weyl tableau.

$$\left(\begin{matrix} \langle\lambda_1\rangle & \langle\lambda_2\rangle \\ & \langle\mu_2\rangle \end{matrix} \middle| \begin{matrix} \langle\lambda\rangle \\ \langle\mu\rangle \end{matrix}\right) = \sum_{\rho_m^2} \frac{N(\lambda, \rho_m^2)}{N(\lambda_2, \tau^2)} \left(\begin{matrix} [\lambda_1] & [\lambda_2] \\ & [\mu_2] \end{matrix} \middle| \begin{matrix} [\lambda] \\ [\mu] \end{matrix}\right)$$

$$= \sum_{\tau^2} \frac{N(\lambda_2, \tau^2)}{N(\lambda, \rho^2)} \left(\begin{matrix} [\lambda_1] & [\lambda_2] \\ & [\mu_2] \end{matrix} \middle| \begin{matrix} [\lambda] \\ [\mu] \end{matrix}\right), \tag{111}$$

where the last relationship results when we start from an inverse of eq. (35). Here, we defined $[\mu_2] \equiv [\lambda_2 - f(\tau^2)]$ and $[\mu] \equiv [\lambda - f(\rho_m^2)]$, which result from the removal of f boxes constituting the partial tableaux τ^2 and ρ_m^2, respectively, from the tableaux $[\lambda_2]$ and $[\lambda]$. Thus, the I_s factors appearing in eq. (111) are in fact the f-particle I_s factors defined, in complete analogy to the multiple I_o factors of eq. (83), as a product of one-particle I_s factors, namely

$$\left(\begin{matrix} [\lambda_1] & [\lambda_2] \\ & [\mu_2] \end{matrix} \middle| \begin{matrix} [\lambda] \\ [\mu] \end{matrix}\right) \equiv \left(\begin{matrix} [\lambda_1] & [\lambda_2] \\ & [\lambda_2 - f(\tau^2)] \end{matrix} \middle| \begin{matrix} [\lambda] \\ [\lambda - f(\rho_m^2)] \end{matrix}\right)$$

$$= \left(\begin{matrix} [\lambda_1] & [\lambda_2] \\ & [\lambda_2 - 1(\tau^2)] \end{matrix} \middle| \begin{matrix} [\lambda] \\ [\lambda - 1(\rho_m^2)] \end{matrix}\right)$$

$$\times \left(\begin{matrix} [\lambda_1] & [\lambda_2 - 1(\tau^2)] \\ & [\lambda_2 - 2(\tau^2)] \end{matrix} \middle| \begin{matrix} [\lambda - 1(\rho_m^2)] \\ [\lambda - 2(\rho_m^2)] \end{matrix}\right)$$

$$\ldots \left(\begin{matrix} [\lambda_1] & [\lambda_2 - (f-1)(\tau^2)] \\ & [\lambda_2 - f(\tau^2)] \end{matrix} \middle| \begin{matrix} [\lambda - (f-1)(\rho_m^2)] \\ [\lambda - f(\rho_m^2)] \end{matrix}\right), \tag{111'}$$

where τ^2 and ρ_m^2 define the sequence in which the f boxes are removed.

We can, finally, transform the I_s factor into the I_o factor using eq. (52) or eq. (53). Exploiting then eq. (101) for this particular case, we can also directly relate the I_t and I_u factors, namely

$$\begin{pmatrix} \langle\lambda_1\rangle & \langle\lambda_2\rangle \\ & \langle\mu_2\rangle \end{pmatrix} \begin{vmatrix} \langle\lambda\rangle \\ \langle\mu\rangle \end{pmatrix} = \frac{\gamma(\lambda_1,\mu_2;\mu)}{\gamma(\lambda_1,\lambda_2;\lambda)} \begin{pmatrix} \langle\lambda_1\rangle & \langle\lambda_2\rangle \\ \langle\lambda_1\rangle & \langle\mu_2\rangle \end{pmatrix} \begin{vmatrix} \langle\lambda\rangle \\ \langle\mu\rangle \end{pmatrix}$$

$$= \left[\frac{N!(N_2-f)!f_\mu f_{\lambda_2}}{(N-f)!N_2!f_{\mu_2}f_\lambda}\right]^{1/2} \begin{pmatrix} \langle\lambda_1\rangle & \langle\lambda_2\rangle \\ \langle\lambda_1\rangle & \langle\mu_2\rangle \end{pmatrix} \begin{vmatrix} \langle\lambda\rangle \\ \langle\mu\rangle \end{pmatrix}, \tag{112}$$

with γ given by eq. (45). Note that when $f = 1$, this relationship is identical with that relating I_s and I_o factors (eq. (52) or eq. (53)).

To conclude, we remark that we now have at our disposal the explicit relationship among all four isoscalar factors I_o, I_s, I_u and I_t. The principal relationships are given by eqs. (53), (101) and (112). In the many-electron case, eqs. (103), (105), (106), (108) and (109) are very useful. Thus, knowing one of the factors, we can now determine all the remaining ones, if needed.

5. Explicit algebraic expressions for isoscalar factors

We shall now present explicit expressions for the isoscalar factors, which are required in UGA formalism, and examine their symmetry properties. We can thus restrict ourselves to at most two-column irreps of U(n), which we again label as indicated in eq. (102). The Kronecker product of two such irreps $\langle 2^a 1^b\rangle \otimes \langle 2^d 1^e\rangle \equiv (a,b) \otimes (d,e)$ can, of course, contain three- and four-column irreps. These, however, can be ignored in many-electron problems, since the corresponding wave functions must vanish in view of the Pauli principle. Assuming that $b \geq e$, we easily find that

$$(a,b) \otimes (d,e) \rightarrow \sum_{k=0}^{k_m} \oplus (a+d+e-k, b-e+2k)$$

$$\rightarrow \sum_{k=k_M}^{e} \oplus (a+d+k, b+e-2k), \tag{113}$$

where

$$k_m = \min\{e, n-(a+b+d)\},$$

$$k_M = \max\{0, a+b+d+e-n\},$$

and the arrow indicates a restriction to at most two-column tableaux. Thus, for example,

$$(2,1) \otimes (1,1) \rightarrow (4,0) \oplus (3,2), \tag{114}$$

assuming that $n \geq 5$. Clearly, if $n = 4$, only the first irrep survives, while for $n \leq 3$, no two-column irreps can be formed. Since usually $n \gg N = 2(a + d) + b + e$ in most quantum chemical computations, we can simply take $k_m = e$ or $k_M = 0$. Clearly, the CG series (113) is dual to the corresponding SU(2) × SU(2) coupling for spins, as may be easily seen from the behavior of the second label in eq. (113).

We recall that a general CG coefficient

$$\left\langle \begin{matrix} (a,b) & (d,e) \\ U & V \end{matrix} \middle| \begin{matrix} (s,t) \\ W \end{matrix} \right\rangle \tag{115}$$

factorizes into a successive product of I_u factors

$$\begin{pmatrix} (a,b) & (d,e) \\ (a',b') & (d',e') \end{pmatrix} \begin{matrix} (s,t) \\ (s',t') \end{matrix} \Big)_u, \tag{116}$$

similarly as given by eq. (50) for the S_N coefficients. Since we now consider only the U(n) factors, for simplicity we can omit the subscript u. Thus, for example (note that we delete the irrep labels in CG coefficients since they are implied by Weyl tableaux)

$$\left\langle \begin{matrix} 1 & 3 & 2 & 6 \\ 2 & 4 & 5 & \\ 7 & & & \end{matrix} \middle| \begin{matrix} 1 & 2 \\ 2 & 4 \\ 3 & 6 \\ 5 & \\ 7 & \end{matrix} \right\rangle = \begin{pmatrix} (2,1) & (1,1) \\ (2,0) & (1,1) \end{pmatrix} \begin{matrix} (3,2) \\ (3,1) \end{matrix} \Big) \cdot \begin{pmatrix} (2,0) & (1,1) \\ (2,0) & (0,2) \end{pmatrix} \begin{matrix} (3,1) \\ (2,2) \end{matrix} \Big)$$

$$\times \begin{pmatrix} (2,0) & (0,2) \\ (2,0) & (0,1) \end{pmatrix} \begin{matrix} (2,2) \\ (2,1) \end{matrix} \Big) \cdot \begin{pmatrix} (2,0) & (0,1) \\ (1,1) & (0,1) \end{pmatrix} \begin{matrix} (2,1) \\ (1,2) \end{matrix} \Big)$$

$$\times \begin{pmatrix} (1,1) & (0,1) \\ (0,2) & (0,1) \end{pmatrix} \begin{matrix} (1,2) \\ (1,1) \end{matrix} \Big) \cdot \begin{pmatrix} (0,2) & (0,1) \\ (0,1) & (0,0) \end{pmatrix} \begin{matrix} (1,1) \\ (0,1) \end{matrix} \Big). \tag{117}$$

There are nine independent possibilities for the I_u factors of the type (116), depending on the orbital occupancies, as shown schematically in fig. 5, including the trivial unoccupied case (diagram O),

$$\begin{pmatrix} (a,b) & (d,e) \\ (a,b) & (d,e) \end{pmatrix} \begin{matrix} (s,t) \\ (s,t) \end{matrix} \Big)_u = 1. \tag{118}$$

The derivation of explicit expressions for these factors is given in the appendix. The results are summarized in table 2. These results generalize those given in our earlier

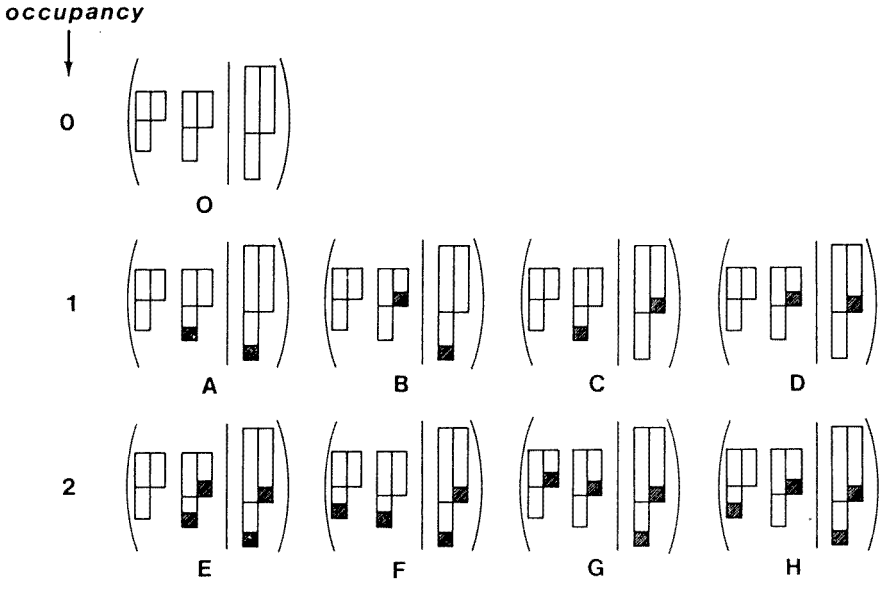


Fig. 5. Schematic representation of basic distinct types of U(n) and S_N isoscalar factors, involving at most two-column irreps of the unitary group approach to many-electron systems. The factors are arranged by the occupancy of the highest orbital, starting with the trivial unoccupied case (O). The remaining factors are obtained by the interchange of the first two tableaux, which brings about the phase change given by eqs. (119)–(121). All tableaux shown pertain to the I_u factors, while the I_o factors of S_N can only involve single occupancies and can thus be of types A–D. For the I_t factors, types O and A–E can occur, while again only types A–D pertain to the I_s factors of S_N. See text for details.

paper [75], which were restricted to the coupling of single-column tableaux, i.e. to the case that $a = d = 0$. The latter can be easily obtained by setting $a = d = 0$ in table 2. For example, case (A) will yield eq. (A9) of [75], taking into account eq. (A2) and the generalized Condon–Shortley phase convention.

We remark that table 2 gives only independent I_u factors, the remaining ones being given by their symmetry properties. We recall [74,75] that an interchange of the first two columns changes only the phase, given by the irreps involved, namely

$$\begin{pmatrix} \langle\lambda\rangle & \langle\mu\rangle & | & \langle\nu\rangle \\ \langle\lambda'\rangle & \langle\mu'\rangle & | & \langle\nu'\rangle \end{pmatrix} = (-1)^{\langle\lambda\rangle+\langle\lambda'\rangle+\langle\mu\rangle+\langle\mu'\rangle+\langle\nu\rangle+\langle\nu'\rangle} \begin{pmatrix} \langle\mu\rangle & \langle\lambda\rangle & | & \langle\nu\rangle \\ \langle\mu'\rangle & \langle\lambda'\rangle & | & \langle\nu'\rangle \end{pmatrix}. \quad (119)$$

For two-column irreps, this phase factor is given by the formulas:

$$(-1)^{(a,b)} = (-1)^{(0,a+b)}(-1)^{(0,a)} = (-1)^{ab+b(b-1)/2}, \quad (120a)$$

since

Table 2

Explicit expressions for isoscalar factors $\begin{pmatrix} (a,b) & (d,e) & (s,t) \\ (a',b') & (d',e') & (s',t') \end{pmatrix}$. Types refer to fig. 5. See text for details

Occupancy	Type	(a',b')	(d',e')	(s',t')	$I_u\,(I_o)$	$I_t\,(I_s)$
0	O	(a,b)	(d,e)	(s,t)	1	1
1	A	(a,b)	$(d,e-1)$	$(s,t-1)$	$\frac{1}{2}\left[\frac{(d+e+1)(b+e+t+2)(e-b+t)}{t(e+1)(s+t+1)}\right]^{1/2}$	$\frac{1}{2}\left[\frac{(b+e+t+2)(e-b+t)}{e(t+1)}\right]^{1/2}$
	B	(a,b)	$(d-1,e+1)$	$(s,t-1)$	$\frac{(-1)^{a+d+e+s}}{2}\left[\frac{d(b-e+t)(b+e+2-t)}{t(e+1)(s+t+1)}\right]^{1/2}$	$\frac{(-1)^{a+d+e+s}}{2}\left[\frac{(b+e+2-t)(b-e+t)}{(e+2)(t+1)}\right]^{1/2}$
	C	(a,b)	$(d,e-1)$	$(s-1,t+1)$	$\frac{(-1)^{a+d+e+s}}{2}\left[\frac{(d+e+1)(e+b-t)(b-e+t+2)}{s(e+1)(t+2)}\right]^{1/2}$	$\frac{(-1)^{a+d+e+s}}{2}\left[\frac{(b+e+t+2)(b+e-t)}{e(t+1)}\right]^{1/2}$
	D	(a,b)	$(d-1,e+1)$	$(s-1,t+1)$	$\frac{1}{2}\left[\frac{d(e-b+t+2)(e+b+t+4)}{s(e+1)(t+2)}\right]^{1/2}$	$\frac{1}{2}\left[\frac{(e-b+t+2)(b+e+t+4)}{(e+1)(t+1)}\right]^{1/2}$
2	E	(a,b)	$(d-1,e)$	$(s-1,t)$	$\left[\frac{d(d+e+1)}{s(s+t+1)}\right]^{1/2}$	1
	F	$(a,b-1)$	$(d,e-1)$	$(s-1,t)$	$\frac{(-1)^{d}}{2}\left[\frac{(a+b+1)(d+e+1)(b+e-t)(b+e+t+2)}{s(s+t+1)(b+1)(e+1)}\right]^{1/2}$	–
	G	$(a-1,b+1)$	$(d-1,e+1)$	$(s-1,t)$	$\frac{(-1)^{d+e}}{2}\left[\frac{ad(b+e+2-t)(b+e+t+4)}{s(s+t+1)(b+1)(e+1)}\right]^{1/2}$	–
	H	$(a,b-1)$	$(d-1,e+1)$	$(s-1,t)$	$\frac{(-1)^{a+b+s+t}}{2}\left[\frac{d(a+b+1)(b-e+t)(e-b+t+2)}{s(s+t+1)(b+1)(e+1)}\right]^{1/2}$	–

$$(-1)^{(0,b)} = (-1)^{b(b-1)/2}. \tag{120b}$$

The following special cases are very useful in actual applications:

$$\begin{aligned}(-1)^{(a,b)+(a,b-1)} &= (-1)^{a+b+1},\\ (-1)^{(a,b)+(a-1,b+1)} &= (-1)^{a+1},\\ (-1)^{(a,b)+(a-1,b)} &= (-1)^{b}.\end{aligned} \tag{121}$$

Using this symmetry property, we easily obtain the remaining I_u factors that are not listed explicitly in table 2.

We can now also obtain the explicit expressions for the remaining isoscalar factors. We know that the I_o factor for S_N equals the corresponding I_u factor when only single occupancies are allowed (eq. (101)). Thus, only those cases are relevant for the I_o factors in which a single box is detached from the Young tableau, i.e. cases (A–D) of fig. 4 and table 2. The I_o factors are in this case given by exactly the same expressions as the I_u factors and, consequently, are not repeated in table 2.

The I_t factors can be similarly obtained using relationship (112). As property (60) indicates, the highest label must always occur in the second Weyl tableau W_2 of the transformation coefficient defined by eq. (59). This is also clear from the structure of the I_t factors, whose first irrep is always the same as the notation of eq. (62) implies. Consequently, only cases (A–E) of fig. 4 can occur for the I_t factors. For the same reason, there is no symmetry property for these factors, although one could formally introduce a similar property as for the I_u factors (eq. (119)) if desired. The relevant explicit expressions for the I_t factors are listed in the last column of table 2.

Finally, the expressions for the I_s factors are again identical with those for the I_t factors. Since only single occupancies are relevant in this case, the pertinent expressions are given by the formulas in the last column of table 2 for cases (A–D).

We now illustrate some possible applications of the derived expressions given in table 2 on a few examples.

Example 1

The CG coefficient appearing on the left-hand side of eq. (117) is easily evaluated to be

$$\left\langle \begin{array}{cccc|cc} 1 & 3 & 2 & 6 & 1 & 2 \\ 2 & 4 & 5 & & 2 & 4 \\ 7 & & & & 3 & 6 \\ & & & & 5 & \\ & & & & 7 & \end{array} \right\rangle = 2^{-1/2}\cdot 3^{-1/2}\cdot (3/5)^{1/2}\cdot 1\cdot (-1/4)\cdot 1 = -4^{-1}\cdot 10^{-1/2}, \tag{122}$$

where we have used the segments of types A, B, D and F.

Example 2

We can couple the irrep bases for $\langle 2\ 1\rangle \equiv (1,1)$ and $\langle 2\rangle \equiv (1,0)$ of U(n) to obtain a basis for the irrep $\langle 2^2 1\rangle \equiv (2,1)$ of U(n), where $n \geq 3$. One of the resulting states will have the form:

$$\left|\begin{matrix}1 & 2\\ 2 & 3\\ 5\end{matrix}\right\rangle = (1/4)\left|\begin{matrix}1 & 2\\ 2\end{matrix}\right\rangle |3\ 5\rangle + (\sqrt{2}/8)\left|\begin{matrix}1 & 2\\ 3\end{matrix}\right\rangle |2\ 5\rangle - (2\sqrt{3}/8)\left|\begin{matrix}1 & 3\\ 2\end{matrix}\right\rangle |2\ 5\rangle$$

$$+ (1/2)\left|\begin{matrix}1 & 3\\ 5\end{matrix}\right\rangle |2\ 2\rangle + (1/2)\left|\begin{matrix}2 & 2\\ 5\end{matrix}\right\rangle |1\ 3\rangle - (\sqrt{2}/4)\left|\begin{matrix}2 & 3\\ 5\end{matrix}\right\rangle |1\ 2\rangle$$

$$- (1/4)\left|\begin{matrix}2 & 2\\ 3\end{matrix}\right\rangle |1\ 5\rangle - (\sqrt{2}/4)\left|\begin{matrix}1 & 2\\ 5\end{matrix}\right\rangle |2\ 3\rangle, \tag{123}$$

since the relevant CG coefficients are easily evaluated as in example 1, e.g.,

$$\left\langle\begin{matrix}1 & 2 & 3 & 5\\ 2\end{matrix}\middle|\begin{matrix}1 & 2\\ 2 & 3\\ 5\end{matrix}\right\rangle = \begin{pmatrix}(1,1) & (1,0)\\ (1,1) & (0,1)\end{pmatrix}\begin{vmatrix}(2,1)\\ (2,0)\end{vmatrix}\cdot\begin{pmatrix}(1,1) & (0,1)\\ (1,1) & (0,0)\end{pmatrix}\begin{vmatrix}(2,0)\\ (1,1)\end{vmatrix}$$

$$= (1/2)\cdot(1/2) = \tfrac{1}{4}, \text{ etc.} \tag{124}$$

We can easily verify that the resulting state (123) is normalized, since the CG coefficients constitute a unitary transformation. Note, however, that for an inverse transformation we obtain, for example,

$$|3\ 5\rangle\left|\begin{matrix}1 & 2\\ 2\end{matrix}\right\rangle = (1/4)\left|\begin{matrix}1 & 2\\ 2 & 3\\ 5\end{matrix}\right\rangle + (\sqrt{3}/4)\left|\begin{matrix}1 & 2\\ 2 & 5\\ 3\end{matrix}\right\rangle, \tag{125}$$

the relevant coefficients again being given by the CG coefficients, e.g. eq. (124). The reason why this inverse relationship appears to be unnormalized can be understood as follows. We can regard the first basis state $|3\ 5\rangle$ as a component of a symmetric tensor operator, which transforms as a basis for the irrep $\langle 2\rangle$, acting on the GT state $\left|\begin{smallmatrix}1 & 2\\ 2\end{smallmatrix}\right\rangle$ of a many-electron system. This will produce two five-electron GT states belonging to the irrep $\langle 2^2 1\rangle$. Generally, however, we must also include basis states belonging to the irreps $\langle 4\ 1\rangle$, $\langle 3\ 2\rangle$ and $\langle 3\ 1^2\rangle$ in addition to the two-column irrep $\langle 2^2 1\rangle$ considered, in which case the normalization condition will hold again. However, these three- and four-column states will vanish for many-electron systems, so that they will not appear on the right-hand side of eq. (125).

Example 3

Using the system partitioning [14,40,83] for the states belonging to the irrep $\langle 2^2 1\rangle$, we can express the states adapted to a chain $U(n_1 + n_2) \supset U(n_1) \otimes U(n_2)$ in terms of $U(n) \equiv U(n_1 + n_2)$ GT states or of their CAUGA representation in the irrep $\langle 2\rangle$ of $U(2^n)$. Thus, considering a partitioned irrep $\langle 2\ 1\rangle \otimes \langle 2\rangle$, we obtain, for example, that

$$\left|\langle 2^2 1\rangle \begin{matrix} 1 & 2 \\ 2 \end{matrix} \quad 3 \quad 5\right\rangle = (1/2)\left|\begin{matrix} 1 & 2 \\ 2 & 3 \\ 5 \end{matrix}\right\rangle + (\sqrt{3}/2)\left|\begin{matrix} 1 & 2 \\ 2 & 5 \\ 3 \end{matrix}\right\rangle, \tag{126}$$

since

$$\left\langle \langle 2^2 1\rangle \begin{matrix} 1 & 2 \\ 2 \end{matrix} \quad 3 \quad 5 \middle| \begin{matrix} 1 & 2 \\ 2 & 3 \\ 5 \end{matrix}\right\rangle = \left(\langle 2\ 1\rangle \quad \begin{matrix} \langle 2\rangle \\ \langle 1\rangle \end{matrix} \middle| \begin{matrix} \langle 2^2 1\rangle \\ \langle 2^2\rangle \end{matrix}\right)\left(\langle 2\ 1\rangle \quad \begin{matrix} \langle 1\rangle \\ \langle 0\rangle \end{matrix} \middle| \begin{matrix} \langle 2^2\rangle \\ \langle 2\ 1\rangle \end{matrix}\right)$$

$$= \left((1,1) \quad \begin{matrix} (1,0) \\ (0,1) \end{matrix} \middle| \begin{matrix} (2,1) \\ (2,0) \end{matrix}\right)_t \left((1,1) \quad \begin{matrix} (0,1) \\ (0,0) \end{matrix} \middle| \begin{matrix} (2,0) \\ (1,1) \end{matrix}\right)_t = (1/2)\cdot 1 = 1/2, \tag{127}$$

and

$$\left\langle \langle 2^2 1\rangle \begin{matrix} 1 & 2 \\ 2 \end{matrix} \quad 3 \quad 5 \middle| \begin{matrix} 1 & 2 \\ 2 & 5 \\ 3 \end{matrix}\right\rangle = \left((1,1) \quad \begin{matrix} (1,0) \\ (0,1) \end{matrix} \middle| \begin{matrix} (2,1) \\ (1,2) \end{matrix}\right)_t \left((1,1) \quad \begin{matrix} (0,1) \\ (0,0) \end{matrix} \middle| \begin{matrix} (2,1) \\ (1,1) \end{matrix}\right)_t$$

$$= (\sqrt{3}/2)\cdot 1 = \sqrt{3}/2, \tag{128}$$

using the I_t factors of types B, C and D, A, respectively. Representing GT states on the right-hand side of eq. (126) in terms of CAUGA two-box states [13–15,75], we will obtain directly the CAUGA representation of the partitioned basis. We can thus generate directly CAUGA partitioned basis states employing the I_t factors of table 2.

It is instructive to note the difference between eqs. (125) and (126), which are very similar at first sight. The first, eq. (125), represents a product state from the irrep $\langle 2\rangle \otimes \langle 2\ 1\rangle$ in terms of GT states carrying the $\langle 2^2 1\rangle$ irrep of $U(n)$, $n \geq 3$. The second, eq. (126), represents a partitioned basis state for the irrep $\langle 2^2 1\rangle$ (i.e. not a GT state adapted to the canonical chain (54), but a non-GT state adapted to the chain (58)), again expressed as a linear combination of GT states carrying the same irrep. Consequently, the latter state is properly normalized since we are within the same irrep.

6. U(*n*) Racah coefficients

We have seen above that, in complete analogy to the SU(2) angular momentum theory, one can introduce various vector coupling coefficients and corresponding

isoscalar factors for both S_N and U(n) groups and interrelate them using the well-known S_N–U(n) reciprocity. Motivated by this analogy, we can similarly introduce Racah recoupling coefficients or corresponding $6j$ symbols when dealing with the coupling of three basis vectors. In the SU(2) case, where no multiplicity problem arises, the usefulness of this concept can hardly be overestimated. We recall that in this case there is a simple relationship between the Racah coefficients W or U (due to Jahn [85]) and $6j$ coefficients, namely

$$\begin{aligned}
&\langle j_1 j_2 (j_{12}), j_3; jm \,|\, j_1, j_2 j_3 (j_{23}); j'm' \rangle \\
&\quad = \delta_{jj'} \cdot \delta_{mm'} U(j_1 j_2 j j_3; j_{12} j_{23}) \\
&\quad = \delta_{jj'} \cdot \delta_{mm'} (-1)^{j_1+j_2+j_3+j} [(2j_{12}+1)(2j_{23}+1)]^{1/2} \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j & j_{23} \end{Bmatrix} \\
&\quad = \delta_{jj'} \cdot \delta_{mm'} [(2j_{12}+1)(2j_{23}+1)]^{1/2} W(j_1 j_2 j j_3; j_{12} j_{23}),
\end{aligned} \tag{129}$$

where $|j_1 j_2 (j_{12}), j_3; jm\rangle$ and $|j_1, j_2 j_3 (j_{23}); jm\rangle$ designate distinct basis vectors obtained by coupling the tensor product basis $|j_1 m_1\rangle |j_2 m_2\rangle |j_3 m_3\rangle$ following the coupling schemes ((1,2),3) and (1,(2,3)), respectively.

The usefulness of U(n) Racah coefficients, which we will now define, will become apparent when we evaluate matrix elements of the products of two tensor operators or when we construct isoscalar factors for nontrivial tensor operators (such as adjoint tensors) from those given in the preceding sections. Although we cannot give here a general treatment, which would enable one to obtain an arbitrary U(n) Racah coefficient, we shall consider a few very useful special classes of these coefficients, in particular those associated with multiplicity-free couplings. We shall also briefly mention some basic properties of these coefficients, which show their similarity to the corresponding SU(2) quantities.

Just as in the angular momentum theory, the U(n) Racah coefficients represent transformation coefficients between the states obtained through different coupling schemes, namely

$$\begin{aligned}
&|(\lambda_1 \lambda_2) \alpha_{12} \lambda_{12}, \lambda_3; \alpha \lambda\rangle \\
&\quad = \sum_{\lambda_{23}, \alpha_{23}, \alpha'} U(\lambda_1 \lambda_2 \lambda \lambda_3; \lambda_{12} \lambda_{23})_{\alpha_{12} \alpha_{23} \alpha \alpha'} |\lambda_1, (\lambda_2 \lambda_3) \alpha_{23} \lambda_{23}; \alpha' \lambda\rangle,
\end{aligned} \tag{130}$$

where we have dropped the angular brackets designating U(n) irreps, writing simply $\langle \lambda_i \rangle \equiv \lambda_i$, and where we introduced multiplicity labels which resolve the multiplicity problem in the following couplings [73]:

$$\lambda_1 \times \lambda_2 \to \alpha_{12}\lambda_{12}, \qquad \lambda_{12} \times \lambda_3 \to \alpha\lambda,$$

$$\lambda_2 \times \lambda_3 \to \alpha_{23}\lambda_{23}, \qquad \lambda_1 \times \lambda_{23} \to \alpha'\lambda. \tag{131}$$

Carrying out the indicated couplings using repeatedly eq. (55), we can express the Racah coefficient U in terms of CG coefficients as follows:

$$\delta_{\lambda\lambda'}\delta_{WW'}U(\lambda_1\lambda_2\lambda\lambda_3;\lambda_{12}\lambda_{23})_{\alpha_{12},\alpha_{23},\alpha,\alpha'} = \sum_{\{W_i\}} \left\langle \begin{matrix} \lambda_1 & \lambda_2 \\ W_1 & W_2 \end{matrix} \middle| \begin{matrix} \alpha_{12}\lambda_{12} \\ W_{12} \end{matrix} \right\rangle$$

$$\times \left\langle \begin{matrix} \lambda_{12} & \lambda_3 \\ W_{12} & W_3 \end{matrix} \middle| \begin{matrix} \alpha\lambda \\ W \end{matrix} \right\rangle \left\langle \begin{matrix} \lambda_2 & \lambda_3 \\ W_2 & W_3 \end{matrix} \middle| \begin{matrix} \alpha_{23}\lambda_{23} \\ W_{23} \end{matrix} \right\rangle \left\langle \begin{matrix} \lambda_1 & \lambda_{23} \\ W_1 & W_{23} \end{matrix} \middle| \begin{matrix} \alpha'\lambda' \\ W' \end{matrix} \right\rangle, \tag{132}$$

where the summation extends over all Weyl tableaux except for the resulting ones $W = W'$. The Racah coefficient U vanishes unless all the couplings (131) satisfy the Littlewood–Richardson rules.

The basic properties of these U(n) Racah coefficients parallel those for the SU(2) ones. In particular, we note the following rules:

(i) Orthogonality properties implied by the unitarity of transformation (130),

$$\sum_{\lambda_{23},\alpha_{23},\alpha'} U(\lambda_1\lambda_2\lambda\lambda_3;\lambda_{12}\lambda_{23})_{\alpha_{12},\alpha_{23},\alpha,\alpha'}U(\lambda_1\lambda_2\lambda\lambda_3;\lambda'_{12}\lambda_{23})_{\alpha'_{12},\alpha_{23},\alpha'',\alpha'}$$

$$= \delta_{\lambda_{12}\lambda'_{12}}\delta_{\alpha_{12},\alpha'_{12}}\delta_{\alpha,\alpha''}, \tag{133a}$$

$$\sum_{\lambda_{12},\alpha_{12},\alpha} U(\lambda_1\lambda_2\lambda\lambda_3;\lambda_{12}\lambda_{23})_{\alpha_{12},\alpha_{23},\alpha,\alpha'}U(\lambda_1\lambda_2\lambda\lambda_3;\lambda_{12}\lambda'_{23})_{\alpha_{12},\alpha'_{23},\alpha,\alpha''}$$

$$= \delta_{\lambda_{23},\lambda'_{23}}\delta_{\alpha_{23},\alpha'_{23}}\delta_{\alpha',\alpha''}\,. \tag{133b}$$

(ii) Out of the numerous symmetry properties, we just note the following one:

$$U(\lambda_1\lambda_2\lambda\lambda_3;\lambda_{12}\lambda_{23})_{\alpha_{12},\alpha_{23},\alpha,\alpha'}$$

$$= \Theta U(\lambda_3\lambda_2\lambda\lambda_1;\lambda_{23}\lambda_{12})_{\alpha_{23},\alpha_{12},\alpha',\alpha}, \tag{134}$$

where the phase factor Θ is given by the product of four phase factors

$$\Theta = \Theta(\lambda_1\lambda_2\lambda_{12})_{\alpha_{12}}\Theta(\lambda_{12}\lambda_3\lambda)_{\alpha}\Theta(\lambda_2\lambda_3\lambda_{23})_{\alpha_{23}}\Theta(\lambda_1\lambda_{23}\lambda)_{\alpha'}, \tag{135}$$

each characterizing the symmetry of corresponding CG coefficients with respect to the interchange of coupled irreps when the coupling is not multiplicity-free, e.g.

$$\left\langle \begin{matrix} \lambda_1 & \lambda_2 \\ W_1 & W_2 \end{matrix} \middle| \begin{matrix} \alpha_{12}\lambda_{12} \\ W_{12} \end{matrix} \right\rangle$$

$$= (-1)^{\lambda_1+\lambda_2+\lambda_{12}} \Theta(\lambda_1\lambda_2\lambda_{12})_{\alpha_{12}} \left\langle \begin{matrix} \lambda_2 & \lambda_1 \\ W_2 & W_1 \end{matrix} \middle| \begin{matrix} \alpha_{12}\lambda_{12} \\ W_{12} \end{matrix} \right\rangle , \tag{136}$$

where the standard phase $(-1)^{\lambda}$ is the same as in eq. (119). In the multiplicity-free case, we thus have that all $\Theta(\lambda_i\lambda_j\lambda_{ij})_{\alpha_{ij}}$ are equal to one so that we recover a standard symmetry property as in the SU(2) case, namely

$$U(\lambda_1\lambda_2\lambda\lambda_3;\lambda_{12}\lambda_{23}) = U(\lambda_3\lambda_2\lambda\lambda_1;\lambda_{23}\lambda_{12}). \tag{137}$$

(iii) Reduction when one of the irreps is a trivial scalar representation $\langle 0\rangle$ gives

$$U(0\lambda_2\lambda_{23}\lambda_3;\lambda_2\lambda_{23})_{-\alpha_{23}\alpha_{23}-} = U(\lambda_1 0\lambda_{13}\lambda_3;\lambda_1\lambda_3)_{--\alpha\alpha}$$

$$= U(\lambda_1\lambda_2\lambda_{12}0;\lambda_{12}\lambda_2)_{\alpha_{12}--\alpha_{12}} = 1. \tag{138}$$

The basic relationship, eq. (132), can be rewritten in several different ways, since we can use the CG orthogonality relations (eqs. (63) and (64)) to move one, two or three CG coefficients to the left-hand side. Thus, multiplying both sides of (132) with

$$\left\langle \begin{matrix} \alpha'\lambda' \\ W' \end{matrix} \middle| \begin{matrix} \lambda_1 & \lambda_{23} \\ W'_1 & W'_{23} \end{matrix} \right\rangle_{\mathrm{u}} ,$$

summing over α', λ' and W', and using relationship (64) (where we now also have to sum over the multiplicity label α'), we obtain

$$\sum_{\alpha'} U(\lambda_1\lambda_2\lambda\lambda_3;\lambda_{12}\lambda_{23})_{\alpha_{12},\alpha_{23},\alpha,\alpha'} \left\langle \begin{matrix} \alpha'\lambda \\ W \end{matrix} \middle| \begin{matrix} \lambda_1 & \lambda_{23} \\ W_1 & W_{23} \end{matrix} \right\rangle_{\mathrm{u}}$$

$$= \sum_{W_2,W_3,W_{12}} \left\langle \begin{matrix} \lambda_1 & \lambda_2 \\ W_1 & W_2 \end{matrix} \middle| \begin{matrix} \alpha_{12}\lambda_{12} \\ W_{12} \end{matrix} \right\rangle_{\mathrm{u}} \tag{139}$$

$$\times \left\langle \begin{matrix} \lambda_{12} & \lambda_3 \\ W_{12} & W_3 \end{matrix} \middle| \begin{matrix} \alpha\lambda \\ W \end{matrix} \right\rangle_{\mathrm{u}} \left\langle \begin{matrix} \lambda_2 & \lambda_3 \\ W_2 & W_3 \end{matrix} \middle| \begin{matrix} \alpha_{23}\lambda_{23} \\ W_{23} \end{matrix} \right\rangle_{\mathrm{u}} ,$$

where in the final expression we dropped the primes on W_1' and W_{23}'. In an analogous manner, we could move two or three CG coefficients to the left-hand side.

We shall now present closely related but new recursion formulas involving U(n) isoscalar factors. Starting with the relationship (139), we first replace the U(n) CG coefficients by the products of I_u factors and U($n-1$) CG coefficients using the definition of isoscalar factors (eq. (56)) which, in the case of general multiplicities, takes the form

$$\left\langle \begin{matrix} \lambda_1 & \lambda_2 \\ W_1 & W_2 \end{matrix} \middle| \begin{matrix} \alpha_{12}\lambda_{12} \\ W_{12} \end{matrix} \right\rangle = \sum_{\beta_{12}} \begin{pmatrix} \lambda_1 & \lambda_2 \\ \mu_1 & \mu_2 \end{pmatrix} \begin{matrix} \alpha_{12}\lambda_{12} \\ \beta_{12}\mu_{12} \end{matrix} \left\langle \begin{matrix} \mu_1 & \mu_2 \\ W_1' & W_2' \end{matrix} \middle| \begin{matrix} \beta_{12}\mu_{12} \\ W_{12}' \end{matrix} \right\rangle , \quad (140)$$

where $\mu_1 \times \mu_2 \rightarrow \beta_{12}\mu_{12}$ are the U($n-1$) irreps and W_1', W_2' and W_{12}' the corresponding U($n-1$) Weyl tableaux. Noting that the summations over W_2, W_3 and W_{12} in eq. (139) now become summations over $\mu_2 W_2'$, $\mu_3 W_3'$ and $\mu_{12} W_{12}'$, and using again eq. (139) for the U($n-1$) to replace the resulting sum over the product of three U($n-1$) CG coefficients by the left-hand side, we finally obtain the desired relationship:

$$\sum_{\alpha'} U(\lambda_1\lambda_2\lambda\lambda_3;\lambda_{12}\lambda_{23})_{\alpha_{12},\alpha_{23},\alpha,\alpha'} \begin{pmatrix} \alpha'\lambda & \lambda_1 & \lambda_{23} \\ \beta'\mu & \mu_1 & \mu_{23} \end{pmatrix}$$

$$= \sum_{\mu_2,\mu_3,\mu_{12}} \sum_{\beta_{12},\beta_{23},\beta} U(\mu_1\mu_2\mu\mu_3;\mu_{12}\mu_{23})_{\beta_{12},\beta_{23},\beta,\beta'} \begin{pmatrix} \lambda_1 & \lambda_2 & \alpha_{12}\lambda_{12} \\ \mu_1 & \mu_2 & \beta_{12}\mu_{12} \end{pmatrix}$$

$$\times \begin{pmatrix} \lambda_{12} & \lambda_3 & \alpha\lambda \\ \mu_{12} & \mu_3 & \beta\mu \end{pmatrix} \begin{pmatrix} \lambda_2 & \lambda_3 & \alpha_{23}\lambda_{23} \\ \mu_2 & \mu_3 & \beta_{23}\mu_{23} \end{pmatrix}. \quad (141)$$

Obviously, for the multiplicity-free case, the sums over α', β_{12}, β_{23} and β are not required. This formula is very useful since it enables us to calculate Racah coefficients recursively by a gradual "dismantelling" of relevant Young tableaux. We shall illustrate its capabilities for a few important special cases in the next section.

7. Expressions for simple U(n) Racah coefficients

Using the recursion formula (141), we can interrelate special classes of U(n) Racah coefficients with U(n) isoscalar factors. We first consider the case where

$$\langle\lambda_1\rangle = \langle 1\rangle, \quad \langle\lambda_2\rangle = \langle m\rangle, \quad \langle\lambda_{12}\rangle = \langle m+1\rangle, \quad (142)$$

so that no multiplicity problem will arise. Choosing, further, $\langle\mu_1\rangle = \langle 0\rangle$, $\langle\mu_{23}\rangle = \langle\lambda_{23}\rangle = \langle\mu\rangle$, we obtain from eq. (141) that

$$U(\langle 1\rangle\langle m\rangle\langle\lambda\rangle\langle\lambda_3\rangle;\langle m+1\rangle\langle\lambda_{23}\rangle)\begin{pmatrix}\langle 1\rangle & \langle\lambda_{23}\rangle & \langle\lambda\rangle \\ \langle 0\rangle & \langle\lambda_{23}\rangle & \langle\lambda_{23}\rangle\end{pmatrix}$$

$$= U(\langle 0\rangle\langle m\rangle\langle\lambda_{23}\rangle\langle\lambda_3\rangle;\langle m\rangle\langle\lambda_{23}\rangle)\begin{pmatrix}\langle 1\rangle & \langle m\rangle & \langle m+1\rangle \\ \langle 0\rangle & \langle m\rangle & \langle m\rangle\end{pmatrix}$$

$$\times\begin{pmatrix}\langle m+1\rangle & \langle\lambda_3\rangle & \langle\lambda\rangle \\ \langle m\rangle & \langle\lambda_3\rangle & \langle\lambda_{23}\rangle\end{pmatrix}\begin{pmatrix}\langle m\rangle & \langle\lambda_3\rangle & \langle\lambda_{23}\rangle \\ \langle m\rangle & \langle\lambda_3\rangle & \langle\lambda_{23}\rangle\end{pmatrix}, \tag{143}$$

since only one term will survive on the right-hand side in view of our choice for μ_1, μ_{23} and μ, which gives $\langle\mu_2\rangle = \langle\mu_{12}\rangle = \langle m\rangle$ and $\langle\mu_3\rangle = \langle\lambda_3\rangle$. The U($n-1$) Racah coefficient now equals one in view of the property (138) and the last isoscalar factor is also trivial and equals one, while the isoscalar factors involving the scalar irrep $\langle 0\rangle$ can be evaluated using eq. (101′), yielding

$$\begin{pmatrix}\langle m\rangle & \langle 1\rangle & \langle m+1\rangle \\ \langle m\rangle & \langle 0\rangle & \langle m\rangle\end{pmatrix} = (m+1)^{-1/2}, \tag{144}$$

$$\begin{pmatrix}\langle\lambda_{23}\rangle & \langle 1\rangle & \langle\lambda\rangle \\ \langle\lambda_{23}\rangle & \langle 0\rangle & \langle\lambda_{23}\rangle\end{pmatrix} = \left(\frac{f_\lambda}{N f_{\lambda_{23}}}\right)^{1/2}, \tag{145}$$

where N gives the number of boxes characterizing the irrep λ. Using the symmetry property (119), we thus obtain

$$U(\langle 1\rangle\langle m\rangle\langle\lambda\rangle\langle\lambda_3\rangle;\langle m+1\rangle\langle\lambda_{23}\rangle) = \left[\frac{N f_{\lambda_{23}}}{(m+1) f_\lambda}\right]^{1/2}\begin{pmatrix}\langle\lambda_3\rangle & \langle m+1\rangle & \langle\lambda\rangle \\ \langle\lambda_3\rangle & \langle m\rangle & \langle\lambda_{23}\rangle\end{pmatrix}, \tag{146}$$

establishing the relationship between the Racah coefficient involving a totally symmetric irrep and the corresponding isoscalar factor.

We can next derive a similar relationship involving totally antisymmetric irreps. In this case, we take

$$\langle\lambda_1\rangle = \langle 1\rangle, \quad \langle\lambda_2\rangle = \langle 1^m\rangle, \quad \langle\lambda_{12}\rangle = \langle 1^{m+1}\rangle, \tag{147}$$

and using a completely analogous procedure, we find

$$U(\langle 1\rangle\langle 1^m\rangle\langle\lambda\rangle\langle\lambda_3\rangle;\langle 1^{m+1}\rangle\langle\lambda_{23}\rangle)$$

$$= \begin{pmatrix} \langle 1^m\rangle & \langle 1\rangle \\ \langle 1^m\rangle & \langle 0\rangle \end{pmatrix} \Bigg| \begin{matrix} \langle 1^{m+1}\rangle \\ \langle 1^m\rangle \end{matrix} \begin{pmatrix} \langle\lambda_3\rangle & \langle 1^{m+1}\rangle \\ \langle\lambda_3\rangle & \langle 1^m\rangle \end{pmatrix} \Bigg| \begin{matrix} \langle\lambda\rangle \\ \langle\lambda_{23}\rangle \end{matrix} \begin{pmatrix} \langle\lambda_{23}\rangle & \langle 1\rangle \\ \langle\lambda_{23}\rangle & \langle 0\rangle \end{pmatrix} \Bigg| \begin{matrix} \langle\lambda\rangle \\ \langle\lambda_{23}\rangle \end{matrix} \Bigg)^{-1}$$

$$= \left[\frac{N f_{\lambda_{23}}}{(m+1) f_\lambda}\right]^{1/2} \begin{pmatrix} \langle\lambda_3\rangle & \langle 1^{m+1}\rangle \\ \langle\lambda_3\rangle & \langle 1^m\rangle \end{pmatrix} \Bigg| \begin{matrix} \langle\lambda\rangle \\ \langle\lambda_{23}\rangle \end{matrix} \Bigg). \tag{148}$$

We can thus evaluate this class of Racah coefficients in terms of isoscalar factors and vice versa, if convenient. For example, taking $m = 1$ and considering at most two-column irreps $\langle 2^a 1^b\rangle = (a, b)$ (eq. (102)), eqs. (146) and (148) provide immediately Racah coefficients for $\langle\lambda_{12}\rangle = \langle 2\rangle$ and $\langle\lambda_{12}\rangle = \langle 1^2\rangle$, respectively, which are given in table 3. These coefficients are very useful in evaluating the matrix elements of symmetric and antisymmetric tensors for many-electron systems, which will be discussed in the second paper of this series.

Table 3

Racah coefficients $U \equiv U(\langle 1\rangle\langle 1\rangle\langle\lambda\rangle\langle 2^a 1^b\rangle;\langle\lambda_{12}\rangle\langle\lambda_{23}\rangle)$ involving symmetric and antisymmetric rank-two tensors $\langle\lambda_{12}\rangle = \langle 2\rangle$ and $\langle 1^2\rangle$, respectively. Shorthand notation (eq. (102)) is employed to label various irreps, $\langle\lambda_3\rangle \equiv \langle 2^a 1^b\rangle \equiv (a, b)$, etc., and we define $\{k, l\} \equiv [(b + k)/(b + l)]^{1/2}$ (cf. eq. (48) of ref. [8])

$\langle\lambda_{12}\rangle$	$\langle\lambda_{23}\rangle$	$\langle\lambda\rangle$	U
(1,0)	$(a,b+1)$	$(a+1,b)$	$\{2,1\}/\sqrt{2}$
	$(a+1,b-1)$	$(a+1,b)$	$\{0,1\}/\sqrt{2}$
(0,2)	$(a,b+1)$	$(a+1,b)$	$-\{0,1\}/\sqrt{2}$
	$(a+1,b-1)$	$(a+1,b)$	$\{2,1\}/\sqrt{2}$
	$(a,b+1)$	$(a,b+2)$	1
	$(a+1,b-1)$	$(a+2,b-2)$	1

Let us finally consider a class of Racah coefficients involving both totally symmetric and antisymmetric irreps. We shall choose

$$\langle\lambda_1\rangle = \langle m\rangle, \ \langle\lambda_3\rangle = \langle 1^k\rangle. \tag{149}$$

Clearly, $\langle\lambda_{12}\rangle$ and $\langle\lambda\rangle$ will result by adding m boxes to $\langle\lambda_2\rangle$ and $\langle\lambda_{23}\rangle$, respectively, so that we can make the following choice for the U($n - 1$) irreps:

$$\langle\mu_1\rangle = \langle 0\rangle, \ \langle\mu_{23}\rangle = \langle\lambda_{23}\rangle = \langle\mu\rangle. \tag{150}$$

Substituting into eq. (141), we thus obtain

$$U(\langle m\rangle\langle\lambda_2\rangle\langle\lambda\rangle\langle 1^k\rangle;\langle\lambda_{12}\rangle\langle\lambda_{23}\rangle)\begin{pmatrix}\langle m\rangle & \langle\lambda_{23}\rangle & | & \langle\lambda\rangle\\ \langle 0\rangle & \langle\lambda_{23}\rangle & | & \langle\lambda_{23}\rangle\end{pmatrix}$$

$$= \sum_{\mu_2,\mu_3,\mu_{12}} U(\langle 0\rangle\langle\mu_2\rangle\langle\lambda_{23}\rangle\langle\mu_3\rangle;\langle\mu_{12}\rangle\langle\lambda_{23}\rangle)\begin{pmatrix}\langle m\rangle & \langle\lambda_2\rangle & | & \langle\lambda_{12}\rangle\\ \langle 0\rangle & \langle\mu_2\rangle & | & \langle\mu_{12}\rangle\end{pmatrix}$$

$$\times\begin{pmatrix}\langle\lambda_{12}\rangle & \langle 1^k\rangle & | & \langle\lambda\rangle\\ \langle\mu_{12}\rangle & \langle\mu_3\rangle & | & \langle\lambda_{23}\rangle\end{pmatrix}\begin{pmatrix}\langle\lambda_2\rangle & \langle 1^k\rangle & | & \langle\lambda_{23}\rangle\\ \langle\mu_2\rangle & \langle\mu_3\rangle & | & \langle\lambda_{23}\rangle\end{pmatrix}. \tag{151}$$

Since in the last factor the resulting irrep $\langle\lambda_{23}\rangle$ does not change when going from U(n) to the U($n-1$) level (eq. (150)), we can immediately conclude that

$$\langle\mu_3\rangle = \langle 1^k\rangle, \quad \langle\mu_2\rangle = \langle\lambda_2\rangle = \langle\mu_{12}\rangle. \tag{152}$$

We can thus rewrite eq. (151) as follows:

$$\begin{pmatrix}\langle\lambda\rangle & \langle 1^k\rangle & | & \langle\nu\rangle\\ \langle\lambda'\rangle & \langle 1^k\rangle & | & \langle\nu'\rangle\end{pmatrix} = (-1)^{\langle\lambda\rangle+\langle\nu\rangle+\langle\lambda'\rangle+\langle\nu'\rangle} U(\langle m\rangle\langle\lambda'\rangle\langle\nu\rangle\langle 1^k\rangle;\langle\lambda\rangle\langle\nu'\rangle)$$

$$\times\begin{pmatrix}\langle\nu'\rangle & \langle m\rangle & | & \langle\nu\rangle\\ \langle\nu'\rangle & \langle 0\rangle & | & \langle\nu'\rangle\end{pmatrix}\begin{pmatrix}\langle\lambda'\rangle & \langle m\rangle & | & \langle\lambda\rangle\\ \langle\lambda'\rangle & \langle 0\rangle & | & \langle\lambda'\rangle\end{pmatrix}^{-1}, \tag{153}$$

where we have relabeled the irreps λ_{12}, λ, λ_2 and λ_{23} as λ, ν, λ' and ν', respectively, to better display the symmetry of this relationship.

The isoscalar factors appearing on the right-hand side of eq. (153) involve the scalar irrep $\langle 0\rangle$ and can be easily evaluated using eq. (101′), similarly as the factors given by eqs. (144) and (145). Thus, for example,

$$\begin{pmatrix}\langle\nu\rangle & \langle m\rangle & | & \langle\lambda\rangle\\ \langle\nu\rangle & \langle 0\rangle & | & \langle\nu\rangle\end{pmatrix} = \left(\frac{f_\lambda m!(N_\lambda - m)!}{f_\nu N_\lambda!}\right)^{1/2}, \tag{154}$$

where N_λ equals the number of boxes in the Young tableau characterizing the irrep $\langle\lambda\rangle$. Substituting into eq. (153), we thus obtain

$$\begin{pmatrix}\langle\lambda\rangle & \langle 1^k\rangle & | & \langle\nu\rangle\\ \langle\lambda'\rangle & \langle 1^k\rangle & | & \langle\nu'\rangle\end{pmatrix} = (-1)^{\langle\lambda\rangle+\langle\nu\rangle+\langle\lambda'\rangle+\langle\nu'\rangle}\left[\frac{f_\nu f_{\lambda'} N_{\nu'}! N_\lambda!}{f_{\nu'} f_\lambda N_\nu! N_{\lambda'}!}\right]^{1/2}$$

$$\times U(\langle m\rangle\langle\lambda'\rangle\langle\nu\rangle\langle 1^k\rangle;\langle\lambda\rangle\langle\nu'\rangle). \tag{155}$$

This formula, in a different form, has recently been derived using the vector coherent state theory [69,70] (cf. eq. (3.12b) of the first ref. [70]). It is clear from our derivation that this result represents a simple recoupling of basis vectors. Moreover, our form shows explicitly the n-independence of this relationship.

8. Conclusions

In this paper, the ground has been laid for the unitary group Racah–Wigner calculus, which is particularly suitable for applications to many-electron systems where at most two-column irreps can occur. After introducing vector coupling coefficients and transformation coefficients between standard (YY or GT) and nonstandard (partitioned) bases for both symmetric (S_N) and unitary [U(n)] groups, we defined corresponding isoscalar factors or reduced Wigner coefficients, in complete analogy to the SU(2) theory. Their usefulness for UGA and CAUGA stems primarily from the fact that the multiplicity problem can be avoided in this case. Using the U(n)–S_N reciprocity of tensor product representations, we were able to interrelate all four distinct isoscalar factors introduced above. It is then convenient to exploit standard S_N representation theory to obtain explicit expressions for all these quantities that are relevant in many-electron problems. We have also considered U(n) Racah coefficients and were able to derive explicit expressions for certain important special classes of these coefficients, which will be useful in evaluation of matrix elements of UGA generators. In all these cases, the Racah coefficients are simply related with the corresponding U(n) isoscalar factors. We shall show in future papers that these factors represent essentially segment level formulas that result from either the heuristic approach of Shavitt [6] or in the SU(2) graphical methods of spin algebra description [8]. When we recall that in the latter approach these segment values are essentially given by the SU(2) 6j coefficients, this is clearly an expected result. However, in this way a clear relationship between the very different derivations is established and a better understanding of the role of the S_N–U(n) reciprocity in the case of many-electron applications is achieved. Moreover, the present approach enables essential simplifications in the treatment of partitioned bases, particularly in the construction of partitioned CAUGA bases and in related problems. It also leads to a rank independent form for important relationships for Racah coefficients that were recently obtained using vector coherent state theory [70]. It should also prove to be very useful in generalizations of present UGA and CAUGA schemes to systems in which electron number and/or total spin-angular momentum are not conserved.

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Appendix

DERIVATION OF EXPLICIT ALGEBRAIC EXPRESSIONS FOR ISOSCALAR FACTORS

In this appendix, we derive the algebraic expressions for the isoscalar factors that are given in section 5. These derivations involve essentially the following three steps: (i) we first reduce the relevant isoscalar factors to the simplest possible form; (ii) we then determine their absolute value using their basic properties such as, for example, their orthogonality relations; (iii) finally, we determine the correct phase factor (using, for example, eq. (23) of ref. [74]) that is consistent with the generalized Condon–Shortley convention for these coefficients [75]. The general properties of these factors, particularly their mutual relationships given by eqs. (53), (101) and (112), immediately imply that we require only the I_o factors (or, equivalently, the I_u factors involving only singly occupied orbitals). However, since all four types of isoscalar factors that we introduced in this paper are simply interrelated, any one of them can be employed in deriving the explicit expressions for them. It turns out that in fact this is most easily done with the I_s or I_t transformation-type factors. Thus, all the distinct types of these factors that we need to evaluate are those listed in fig. 5. The types A–D (fig. 5) are pertinent for both factors, while type E pertains only to the I_t factors.

(1) *Simplification of I_s factors*

Since the values of isoscalar factors are independent of the actual Weyl or Young tableaux involved and depend only on relevant irreps, we can choose arbitrarily the vectors being coupled, or corresponding coupling coefficients, in evaluating these factors, using the basic definitions (eqs. (49), (51), (56) or (62)). Consider, thus, a transformation between canonical GT states and nonstandard partitioned states (eq. (59)) for two-column irreps $\langle 2^a 1^b \rangle \equiv (a, b)$. We shall make a special choice of the $U(n_1)$ and $U(n_2)$ states in which all orbital labels appearing in the two-column part of the Weyl tableau are doubly occupied. We can thus write

$$\left| (s,t) \begin{matrix} (a,b) & (d,e) \\ W_1 & W_2 \end{matrix} \right\rangle = \sum_{\substack{i_1,\dots \\ j_1,\dots}} \left\langle \begin{matrix} (s,t) \\ W \end{matrix} \middle| \begin{matrix} (a,b) & (d,e) \\ W_1 & W_2 \end{matrix} \right\rangle \left| \begin{matrix} (s,t) \\ W \end{matrix} \right\rangle, \tag{A.1}$$

with the Weyl tableaux W_1, W_2 and W having the form:

$$W_1 = \begin{matrix} 1 & 1 \\ \vdots & \vdots \\ a & a \\ a+1 & \\ \vdots & \\ a+b & \end{matrix}, \quad W_2 = \begin{matrix} m+1 & m+1 \\ \vdots & \vdots \\ m+d & m+d \\ m'+1 & \\ \vdots & \\ m'+e & \end{matrix} \tag{A.1'}$$

and

$$W = \begin{array}{ll} 1 & 1 \\ \vdots & \vdots \\ a & a \\ a+1 & m+1 \\ \vdots & \vdots \\ a+b & \\ & m+d \\ m+1 & \\ \vdots & j_1 \\ m+d & \vdots \\ i_1 & \\ \vdots & \end{array}, \qquad \text{(A.1″)}$$

where $m \geq a + b$ and $m' = m + d$, and the sets of labels $\{i_1 \ldots j_1 \ldots\} = \{m' + 1, \ldots, m' + e\}$ are identical. The non-coincidence of boxes in the first and second column of the Weyl tableau that labels the U(n) irrep (s, t) (eq. (A.1″)) schematically expresses the fact that their relative positions cannot be given in general. The maximal label in eq. (A.1) is obviously $m' + e = m + d + e$. Since the doubly-occupied orbitals will not generally change the transformation properties of GT states, the relationship (A.1) will in fact be equivalent to a simpler transformation in which the doubly-occupied parts of each state are removed, namely

$$\left|(s-a-d,t) \quad \begin{matrix}(0,b) & (0,e)\\ W_1' & W_2'\end{matrix}\right\rangle$$

$$= \sum_{\substack{i_1 \ldots \\ j_1 \ldots}} \left\langle \begin{matrix}(s-a-d,t)\\ W'\end{matrix} \middle| \begin{matrix}(0,b) & (0,e)\\ W_1' & W_2'\end{matrix}\right\rangle \left| \begin{matrix}(s-a-d,t)\\ W'\end{matrix}\right\rangle, \qquad \text{(A.2)}$$

where now

$$W_1' = \begin{array}{l} a+1 \\ \vdots \\ a+b \end{array}, \quad W_2' = \begin{array}{l} m'+1 \\ \vdots \\ m'+e \end{array},$$

and

$$W' = \begin{matrix} a+1 & j_1 \\ \vdots & \vdots \\ a+b & \\ i_1 & \\ \vdots & \\ \end{matrix}$$

Consequently, the transformation coefficients in eqs. (A.1) and (A.2) are identical, up to possibly a phase factor Θ, i.e.

$$\left\langle \begin{matrix} (a,b) & (d,e) \\ W_1 & W_2 \end{matrix} \middle| \begin{matrix} (s,t) \\ W \end{matrix} \right\rangle = \Theta \left\langle \begin{matrix} (0,b) & (0,e) \\ W_1' & W_2' \end{matrix} \middle| \begin{matrix} (s-a-d,t) \\ W' \end{matrix} \right\rangle . \tag{A.3}$$

This fact can be best understood by recalling the Clifford algebra representation of canonical GT states [75,86]. Taking now the ratio of two transformation coefficients and using the relationship (A.3), we find that the corresponding isoscalar factors are identical, i.e.

$$\left(\begin{matrix} (a,b) & (d,e) \\ & (d,e-1) \end{matrix} \middle| \begin{matrix} (s,t) \\ (s,t-1) \end{matrix} \right)_s = \left(\begin{matrix} (0,b) & (0,e) \\ & (0,e-1) \end{matrix} \middle| \begin{matrix} (s-a-d,t) \\ (s-a-d,t-1) \end{matrix} \right)_s , \tag{A.4}$$

since the phase factor Θ cancels out. Likewise, we can find a simplified form for the remaining types of the I_s factors (cf. B–D of fig. 5), i.e.

$$\left(\begin{matrix} (a,b) & (d,e) \\ & (d-1,e+1) \end{matrix} \middle| \begin{matrix} (s,t) \\ (s,t-1) \end{matrix} \right)_s$$

$$= \left(\begin{matrix} (0,b) & (1,e) \\ & (0,e+1) \end{matrix} \middle| \begin{matrix} (s-a-d+1,t) \\ (s-a-d+1,t-1) \end{matrix} \right)_s , \tag{A.5}$$

$$\left(\begin{matrix} (a,b) & (d,e) \\ & (d,e-1) \end{matrix} \middle| \begin{matrix} (s,t) \\ (s-1,t+1) \end{matrix} \right)_s$$

$$= \left(\begin{matrix} (0,b) & (0,e) \\ & (0,e-1) \end{matrix} \middle| \begin{matrix} (s-a-d,t) \\ (s-a-d-1,t+1) \end{matrix} \right)_s , \tag{A.6}$$

$$\left(\begin{matrix}(a,b) & (d,e) \\ & (d-1,e+1)\end{matrix}\,\middle|\,\begin{matrix}(s,t) \\ (s,t-1)\end{matrix}\right)_s$$

$$=\left(\begin{matrix}(0,b) & (1,e) \\ & (0,e+1)\end{matrix}\,\middle|\,\begin{matrix}(s-a-d+1,t) \\ (s-a-d,t+1)\end{matrix}\right)_s. \tag{A.7}$$

Now, for cases A and C, the relevant isoscalar factors reduce to a simple case involving couplings of single-column irreps that were considered in our earlier paper [75]. Using the relationship between the I_o and I_s factors (eqs. (52) and (53)), we can translate eqs. (A.4) and (A.6) into the relationship between the corresponding I_o factors and using the results of ref. [75], we find the following expressions for the I_o factors (or, equivalently, I_u factors) of types A and C (fig. 5), namely

$$\left(\begin{matrix}(a,b) & (d,e) \\ (a,b) & (d,e-1)\end{matrix}\,\middle|\,\begin{matrix}(s,t) \\ (s,t-1)\end{matrix}\right)=\left[\frac{(d+e+1)(b+e+t+2)(e-b+t)}{4t(e+1)(s+t+1)}\right]^{1/2}, \tag{A.8}$$

$$\left(\begin{matrix}(a,b) & (d,e) \\ (a,b) & (d,e-1)\end{matrix}\,\middle|\,\begin{matrix}(s,t) \\ (s-1,t+1)\end{matrix}\right)$$

$$=(-1)^{a+e+d+s}\left[\frac{(d+e+1)(b-e+t+2)(e+b-t)}{4s(e+1)(t+2)}\right]^{1/2}, \tag{A.9}$$

where $s \geq a + d$.

While the simplification as expressed through eqs. (A.4)–(A.7) led directly to the desired expressions in cases A and C, the remaining cases B and D require a special treatment, since we cannot eliminate two-column irreps as in the cases A and C. We shall evaluate these factors in the following subsection, considering first the I_o factors corresponding to simplified right-hand sides of eqs. (A.5) and (A.7). Again using the relationships between I_o and I_s factors (eqs. (52) or (53)), we will obtain the desired final expressions.

(2) *Determination of the absolute value*

The absolute values of the remaining isoscalar factors of types B and D (fig. 5), i.e.

$$\left(\begin{matrix}(0,b) & (1,e) \\ (0,b) & (0,e+1)\end{matrix}\,\middle|\,\begin{matrix}(r+1,t) \\ (r+1,t-1)\end{matrix}\right), \tag{A.10b}$$

and

$$\begin{pmatrix}(0,b) & (1,e) \\ (0,b) & (0,e+1)\end{pmatrix}\begin{vmatrix}(r+1,t)\\(r,t+1)\end{vmatrix}, \tag{A.10d}$$

with

$$r \equiv s - a - d, \tag{A.10}$$

can be easily determined from the normalization condition for the I_o or I_u factors (eqs. (65) and (66)). Thus, for example, we obtain:

$$\begin{pmatrix}(0,b) & (1,e) \\ (0,b) & (0,e+1)\end{pmatrix}\begin{vmatrix}(r+1,t)\\(r+1,t-1)\end{vmatrix}^2 + \begin{pmatrix}(0,b) & (1,e) \\ (0,b) & (1,e-1)\end{pmatrix}\begin{vmatrix}(r+1,t)\\(r+1,t-1)\end{vmatrix}^2$$

$$+\begin{pmatrix}(0,b) & (1,e) \\ (0,b-1) & (1,e)\end{pmatrix}\begin{vmatrix}(r+1,t)\\(r+1,t-1)\end{vmatrix}^2 = 1. \tag{A.11}$$

Since the second and third terms on the left-hand side are already known and can be evaluated using eqs. (A.8) and (A.9), we find that

$$\begin{pmatrix}(0,b) & (1,e) \\ (0,b) & (0,e+1)\end{pmatrix}\begin{vmatrix}(r+1,t)\\(r+1,t-1)\end{vmatrix} = \Theta_B\left[\frac{(b+e+2-t)(b+t-e)}{2t(e+1)(b+e+t+4)}\right]^{1/2}, \tag{A.12}$$

where we have used the fact that

$$2r + t = b + e. \tag{A.13}$$

Similarly, we find for the D-type factors

$$\begin{pmatrix}(0,b) & (1,e) \\ (0,b) & (0,e+1)\end{pmatrix}\begin{vmatrix}(r+1,t)\\(r,t+1)\end{vmatrix} = \Theta_D\left[\frac{(b+e+t+4)(e-b+t+2)}{2(e+1)(t+2)(b+e-t+2)}\right]^{1/2}. \tag{A.14}$$

Combining these results with the relationships (A.5) and (A.7), we obtain the desired I_o or I_u factors for cases B and D. It remains to determine their phases Θ_B and Θ_D.

(3) *Determination of phase factors*

The determination of phase factors is more laborious than the determination of absolute values. This is also the case in other approaches [62], which give only the absolute values of reduced Wigner coefficients and require additional considerations

(and conventions) to fix uniquely their phases. In the present case, we shall rely heavily on the recursion relationship, eq. (23) of ref. [74], which uniquely determines the phases once the generalized Condon–Shortley convention is adopted. When we use this relationship in our case (cf. also eq. (A.14) of ref. [75]), we find that

$$\operatorname{sgn}\left(\begin{matrix}(0,b) & (1,e) \\ (0,b) & (0,e+1)\end{matrix}\,\middle|\,\begin{matrix}(r+1,t) \\ (r+1,t-1)\end{matrix}\right)\cdot\operatorname{sgn}\left(\begin{matrix}(0,b) & (1,e) \\ (0,b) & (1,e-1)\end{matrix}\,\middle|\,\begin{matrix}(r+1,t) \\ (r,t+1)\end{matrix}\right)$$

$$=\operatorname{sgn}\left(\begin{matrix}(0,b) & (0,e+1) \\ (0,b) & (0,e)\end{matrix}\,\middle|\,\begin{matrix}(r+1,t-1) \\ (r,t)\end{matrix}\right)\cdot\operatorname{sgn}\left(\begin{matrix}(0,b) & (1,e-1) \\ (0,b) & (0,e)\end{matrix}\,\middle|\,\begin{matrix}(r,t+1) \\ (r,t)\end{matrix}\right), \tag{A.15}$$

where sgn A designates the sign of A, $A = \operatorname{sgn}A \cdot |A|$. Since the second factor on the left-hand side and the first factor on the right-hand side are determined by eq. (A.9), eq. (A.15) yields:

$$\Theta_{\mathrm{B}} = \operatorname{sgn}\left(\begin{matrix}(0,b) & (1,e) \\ (0,b) & (0,e+1)\end{matrix}\,\middle|\,\begin{matrix}(r+1,t) \\ (r+1,t-1)\end{matrix}\right)=\operatorname{sgn}\left(\begin{matrix}(0,b) & (1,e-1) \\ (0,b) & (0,e)\end{matrix}\,\middle|\,\begin{matrix}(r,t+1) \\ (r,t)\end{matrix}\right)$$

$$=\ldots=\operatorname{sgn}\left(\begin{matrix}(0,b) & (1,e-r) \\ (0,b) & (0,e-r+1)\end{matrix}\,\middle|\,\begin{matrix}(1,t+r) \\ (1,t+r-1)\end{matrix}\right), \tag{A.16}$$

using repeatedly the first equation. Before we make a definite determination of this phase factor, we first consider the second one, Θ_{D}. We find similarly that

$$\Theta_{\mathrm{D}} = \operatorname{sgn}\left(\begin{matrix}(0,b) & (1,e) \\ (0,b) & (0,e+1)\end{matrix}\,\middle|\,\begin{matrix}(r+1,t) \\ (r,t+1)\end{matrix}\right)=\operatorname{sgn}\left(\begin{matrix}(0,b) & (1,e-1) \\ (0,b) & (0,e)\end{matrix}\,\middle|\,\begin{matrix}(r+1,t-1) \\ (r,t)\end{matrix}\right)$$

$$=\ldots=\operatorname{sgn}\left(\begin{matrix}(0,b) & (1,r) \\ (0,b) & (0,r+1)\end{matrix}\,\middle|\,\begin{matrix}(r+1,b-r) \\ (r,b-r+1)\end{matrix}\right), \tag{A.17}$$

again using (A.13) in the last step. We cannot continue this recursion any further, since the next isoscalar factor must vanish, i.e.

$$\left(\begin{matrix}(0,b) & (1,r-1) \\ (0,b) & (0,r)\end{matrix}\,\middle|\,\begin{matrix}(r+1,b-r-1) \\ (r,b-r)\end{matrix}\right)=0, \tag{A.18}$$

since the top row coupling violates Littlewood–Richardson rules. We thus invoke the extended Condon–Shortley convention (cf. also eqs. (21a,b) of ref. [75]), requiring that the last nonvanishing isoscalar factor is positive, i.e.

$$\left(\begin{matrix}(0,b) & (1,r) \\ (0,b) & (0,r+1)\end{matrix}\,\middle|\,\begin{matrix}(r+1,b-r) \\ (r+1,b-r-1)\end{matrix}\right) > 0. \tag{A.19}$$

Using again eq. (23) of ref. [74], we obtain:

$$\begin{aligned}
&\mathrm{sgn}\left(\begin{matrix}(0,b) & (1,r) \\ (0,b) & (0,r+1)\end{matrix}\,\middle|\,\begin{matrix}(r+1,b-r) \\ (r,b-r+1)\end{matrix}\right)\cdot \mathrm{sgn}\left(\begin{matrix}(0,b) & (1,r) \\ (0,b) & (0,r+1)\end{matrix}\,\middle|\,\begin{matrix}(r+1,b-r) \\ (r+1,b-r-1)\end{matrix}\right) \\
&\quad = \mathrm{sgn}\left(\begin{matrix}(0,b) & (0,r+1) \\ (0,b) & (0,r)\end{matrix}\,\middle|\,\begin{matrix}(r,b-r+1) \\ (r,b-r)\end{matrix}\right) \\
&\quad \times \mathrm{sgn}\left(\begin{matrix}(0,b) & (0,r+1) \\ (0,b) & (0,r)\end{matrix}\,\middle|\,\begin{matrix}(r+1,b-r-1) \\ (r,b-r)\end{matrix}\right).
\end{aligned} \tag{A.20}$$

Now, the right-hand side factors are of the single-column type and are known from ref. [75] (note that they are of types (iiia) and (iva), fig. 1 of [75]), while the second factor on the left-hand side is fixed by the convention made, eq. (A.19). We thus obtain that

$$\Theta_{\mathrm{D}} = \mathrm{sgn}\left(\begin{matrix}(0,b) & (1,r) \\ (0,b) & (0,r+1)\end{matrix}\,\middle|\,\begin{matrix}(r+1,b-r) \\ (r,b-r+1)\end{matrix}\right) = 1, \tag{A.21}$$

so that $\Theta_{\mathrm{D}} = 1$ independently of the irreps involved.

It thus remains to establish a relationship between Θ_{B} and Θ_{D} factors. Invoking again eq. (23) of [74], we can write similarly to eq. (A.20) that

$$\begin{aligned}
&\mathrm{sgn}\left(\begin{matrix}(0,b) & (1,u) \\ (0,b) & (0,u+1)\end{matrix}\,\middle|\,\begin{matrix}(1,b+u) \\ (1,b+u-1)\end{matrix}\right)\cdot \mathrm{sgn}\left(\begin{matrix}(0,b) & (1,u) \\ (0,b) & (0,u+1)\end{matrix}\,\middle|\,\begin{matrix}(1,b+u) \\ (0,b+u+1)\end{matrix}\right) \\
&\quad = \mathrm{sgn}\left(\begin{matrix}(0,b) & (0,u+1) \\ (0,b) & (0,u)\end{matrix}\,\middle|\,\begin{matrix}(1,b+u+1) \\ (0,b+u)\end{matrix}\right) \\
&\quad \times \mathrm{sgn}\left(\begin{matrix}(0,b) & (0,u+1) \\ (0,b) & (0,u)\end{matrix}\,\middle|\,\begin{matrix}(0,b+u-1) \\ (0,b+u)\end{matrix}\right),
\end{aligned} \tag{A.22}$$

where the right-hand side factors are again of types (iiia) and (iva), fig. 1 of [75], and yield $(-1)^u$. Since the second factor on the left-hand side is of the D-type, while the first one defines Θ_{B} in view of eq. (A.16), with $u = e - r$, we can rewrite eq. (A.22) as

$$\Theta_B \cdot \Theta_D = (-1)^u, \tag{A.23}$$

so that in view of eq. (A.21), we finally obtain that

$$\Theta_B = (-1)^u = (-1)^{e-r} = (-1)^{a+d+e+s}, \tag{A.24}$$

since a, b, d, e and s, t are integers.

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